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NEWS	2	JUL	28	CA/CAplus patent coverage enhanced
NEWS	3	JUL	28	EPFULL enhanced with additional legal status
				information from the epoline Register
NEWS		JUL		IFICDB, IFIPAT, and IFIUDB reloaded with enhancements
NEWS		JUL		STN Viewer performance improved
NEWS		AUG		INPADOCDB and INPAFAMDB coverage enhanced
NEWS	7	AUG	13	CA/CAplus enhanced with printed Chemical Abstracts page images from 1967-1998
NEWS	8	AUG	15	CAOLD to be discontinued on December 31, 2008
NEWS		AUG		CAplus currency for Korean patents enhanced
NEWS	10	AUG	27	CAS definition of basic patents expanded to ensure
				comprehensive access to substance and sequence
				information
NEWS	11	SEP	18	Support for STN Express, Versions 6.01 and earlier,
				to be discontinued
NEWS	12	SEP	25	CA/CAplus current-awareness alert options enhanced
				to accommodate supplemental CAS indexing of
NEWS	1.2	CER	20	exemplified prophetic substances
NEWS	13	SEP	26	WPIDS, WPINDEX, and WPIX coverage of Chinese and and Korean patents enhanced
NEWS	2.4	SEP	20	IFICLS enhanced with new super search field
NEWS		SEP		EMBASE and EMBAL enhanced with new search and
MEMO	13	SEE	23	display fields
NEWS	16	SEP	3.0	CAS patent coverage enhanced to include exemplified
112110		011	-	prophetic substances identified in new Japanese-
				language patents
NEWS	17	OCT	07	
NEWS	18	OCT	07	Multiple databases enhanced for more flexible patent
				number searching
NEWS	19	OCT	22	Current-awareness alert (SDI) setup and editing
				enhanced
NEWS	20	OCT	22	
				Applications
NEWS	21	OCT	24	
				pre-registered REACH substances
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			AND	CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.
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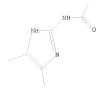
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L4 22 L3

=> s 14 and py<=2004 25113423 PY<=2004

L5 16 L4 AND PY<=2004

=> d 15 1-16 ibib ab hitstr

L5 ANSWER 1 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:836594 CAPLUS

DOCUMENT NUMBER: 139:323523

TITLE: Preparation of aryloxycarbamoylazoles as calcium

channel blockers
INVENTOR(S): Snutch, Terrance P.

PATENT ASSIGNEE(S): Can.

SOURCE: U.S. Pat. Appl. Publ., 22 pp.

CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.
US 20030199523 PRIORITY APPIN. INFO.:	A1	20031023	US 2003-377090 US 2002-360917P
OTHER SOURCE(S):	MARPAT	139:323523	05 2002-300917F

AB ArXQ, Ar2CHXQ [Ar = 6-membered (substituted) aryl containing ≥1 S, O and N, optionally coupled through O to the linker X; X = (substituted) alkylene of 2-10 sequentially connected atoms selected from C, N, O, and S; Q = 5-membered (substituted) heterocyclyl containing ≥1 N or S

atom], were prepared Thus, O-benzotriazolyl-N,N,N',N'-tetramethyluronium tetrafluoroborate was added to a solution of 2-(4,4'-dichlorobenzhydryl)acetic acid, 2-amino-5-nitrothiazole, and Et3N

DATE ------20030228 <---20020228

in CH2C12/MeCN and the reaction mixture was stirred at room temperature overnight to give N-2-(5-nitrothiazoly1)-2-(4,4'-dichlorobenzhydry1)acetic amide (NT

to give N-2-(5-nitrotniazolyl)-Z-(4,4'-dichloropenzhydryl)acetic amide (N: 051). NT 051 blocked α 1B, α 1A, and α 1C channels with IC50 = 0.13 μ M, 6.8 μ M, and 1.91 μ M, resp.

615283-83-5

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of aryloxycarbamoylazoles as calcium channel blockers)

RN 615283-83-5 CAPLUS

CN Acetamide, 2-(2,4-dichlorophenoxy)-N-(4,5-dicyano-1H-imidazol-2-yl)- (CA INDEX NAME)

L5 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2003:532641 CAPLUS DOCUMENT NUMBER: 139:101147

TITLE:

reference

Preparation of aromatic hydrocarbon-fused heterocyclic dithiols and disulfides as electron-accepting compounds capable of forming self-assembled monolayers

INVENTOR(S): Saso, Haruo; Satoh, Toshiaki; Takahashi, Toshiaki;
Ogawa, Satoshi; Yoshimoto, Noriyuki

PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan

SOURCE: PCT Int. Appl., 54 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

	PATENT NO.						KIND DATE			APPLICATION NO.					DATE			
WO 20	030558	53		A1		2003	0710		WO 2	002-	JP13	590		2	0021	226 <	_	
T-	: AE,	AG,	AL,	AM,	ΑT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,		
	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
	GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,		
	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	NZ,	OM,	PH,		
	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	TZ,		
	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	zw								
F	RW: GH,	GM,	KE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,		
	KG,	ΚZ,	MD,	RU,	ΤJ,	TM,	ΑT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,		
	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	SI,	SK,	TR,	BF,	BJ,		
		CG,																
AU 20	AU 2002357515					2003	0715									226 <	-	
PRIORITY F	PRIORITY APPLN. INFO.:								JP 2001-394984					A 20011226				
												5						
									WO 2	002-	JP13	590		W 2	0021	226		

OTHER SOURCE(S): MARPAT 139:101147

The compds. represented by the general formula A-Sp-X [wherein A is (i) an aromatic heterocyclic group bearing at least one member selected from the group consisting of cyano, C1-6 alkoxycarbonyl, and C1-11 acyl either on the ring or in a state attached to the ring through a conjugated system or (ii) an electron-accepting functional group to which at least one aromatic hydrocarbon ring is fused; Sp is a divalent connecting group containing an arylene group and/or an alkylene group; and X is a binding group capable of making a connection to a metal surface, a metal oxide surface, or a semiconductor surface by a covalent or coordinate bond | are prepared | These Compds. have simple structures and are easy of preparation and have the ability to accept an electron and can be self-assembled to form monolayers easily. They are useful as raw materials for mol. devices. Thus, a mixture of naphthalene-1, 4, 5, 8-tetracarboxylic acid dianhydride 5.36, 5-hydroxy-1-pentylamine 4.54, p-toluenesulfonic acid 0.19 g, and 100 mL toluene was refluxed for 8 h with removing H2O though a Dean Stark trap to give 87% N,N'-bis(5-hydroxypentyl)-1,4,5,8-naphthalenetetracarboxylic diimide (I). I (2.02 g) and 3.26 g PBr3 were refluxed in the presence of a catalytic amount of pyridine in 100 mL toluene for 7 h to give 2.65 g crude N, N'-bis(5-bromopentyl)-1, 4, 5, 8-naphthalenetetracarboxylic diimide which was dissolved in 50 mL CHCl3, successively treated with 1.66 q Bu4NBr and aqueous solution of 1.30 g potassium thiosulfate in 20 mL H2O and stirred at room temperature for 25 h to give 81% N, N'-bis(5-acetylthiopentyl)-1, 4, 5, 8-naphthalenetetracarboxylic diimide (II). II (3.21 g) was suspended in 100 MeOH, treated with 10 mL concentrated HCl, and heated under refluxed for 7 days to give 29% N,N'-bis(5-mercaptopentyl)-1,4,5,8-naphthalenetetracarboxylic diimide (III). A gold electrode (1.6 mm diameter) for cyclic voltammetry was immersed in 0.1 mM III/EtOH for 24 h, and successively washed with ethanol and MeCN. A reduction potential of -1.33 V was observed using a Ag/AgNO3

electrode and a Pt electrode against the gold electrode prepared above, which confirmed the formation of a thin film on the gold surface.

556815-13-5P

REFERENCE COUNT:

RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of aromatic hydrocarbon-fused heterocyclic dithiols and disulfides

as electron-accepting compds. capable of forming self-assembled monolavers)

556815-13-5 CAPLUS

CN 1,2-Dithiolane-3-hexanamide, N-(4,5-dicyano-1H-imidazol-2-yl)- (CA INDEX NAME)

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

7 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:888725 CAPLUS

DOCUMENT NUMBER: 137:384838

TITLE: Heterocycle-substituted amides as protease inhibitors INVENTOR(S): Cardel, Bettina; Metz, Guenther; Ottleben, Holger;

THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS

Rau, Harald; Schellhaas, Nathalie; Sekul, Renate; Vetter, Dirk; Bode, Wolfram; Friedrich, Rainer

PATENT ASSIGNEE(S): Graffinity Pharmaceuticals A.-G., Germany

SOURCE: PCT Int. Appl., 180 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PRT

	PATENT NO.					KIND DATE			APPLICATION NO.									
					A1		2002	1121									515 <	
	W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
		co,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,	
		PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	TZ,	
		UA,	UG,	US,	UZ,	VN,	YU,	ZA,	ZM,	ZW								
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AT,	BE,	CH,	
		CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	
		BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG	
DE	1012	4041			A1		2002	1121		DE 2	001-	1012	4041		2	0010	516 <	
AU	2002	3046	30		A1		2002	1125		AU 2	002-	3046	30		2	0020	515 <	
EP	1387	833			A1		2004	0211		EP 2	002-	7327	16		2	0020	515 <	
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
		IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR							
RIT:	ITY APPLN. INFO.:									DE 2	001-	1012	4041		A 2	0010	516	
										WO 2	002-	EP53	69	1	N 2	0020	515	

OTHER SOURCE(S): MARPAT 137:384838 AB ADCR1R2COXCHYEZ [A = (un)substituted aryl, cycloalkyl, cycloalkenyl; D = O, S, S(0), SO2; Rl, R2 = NO2, (un) substituted alkyl, alkoxy, acyl, alkoxycarbonyl, acyloxy, NH2, CONH2, cycloalkyl, aryl, benzyl; X = 0, S, (un) substituted NH; Y = (un) substituted aryl, cycloalkyl, cycloalkenyl, alkyl, alkoxy, acyl; E, Z = H, F, Cl, Br, I, CH, SH, CF3, NO2, acyl, (un) substituted CO2H, acyloxy, alkyl, alkoxy, NH2, CONH2, aryl, cycloalkyl, cycloalkenyl; EZ = (un) substituted CONH2] were prepared for use as inhibitors of proteases, sepecially serine proteases such

as

thrombin. Thus, the diamide I was prepared from polymer-supported 4-H2NSO2C6H4COZH, N-9-fluorenylmethoxycarbonyl-L-4-thiazolylalanine, 4-ClC6H4SCH2COZH, and histamine by solid-phase synthesis. I had Ki for inhibition of thrombin activity of 6X10-6 M.

IT 475680-12-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (USes)

(preparation of heterocycle-substituted amides as inhibitors of thrombin and factor X)

RN 475680-12-7 CAPLUS

CN 4-Thiazolepropanamide, α-[[2-[(4-chlorophenyl)thio]acetyl]amino]-N-(4,5-dicyano-1H-imidazol-2-yl)-, (αS)- (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 4 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:855867 CAPLUS

DOCUMENT NUMBER: 139:214346

TITLE: Product class 3: imidazoles

AUTHOR(S): Grimmett, M. R.

CORPORATE SOURCE: Organic Chemistry, Dept. of Chemistry, University of

Otago, Dunedin, N. Z. Science of Synthesis (2002), 12, 325-528

SOURCE: Science of Synthesis (2002), 12, 325-52 CODEN: SSCYJ9

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

ONGE: ENGIISH

B A review. Methods for preparing imidazoles are reviewed including cyclization, ring transformations, aromatization and modification of substituents on existing imidazoles.

IT 40639-97-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of imidazoles via cyclization, ring transformation,

aromatization and substituent modifications)

RN 40639-97-2 CAPLUS

REFERENCE COUNT:

FORMAT

THERE ARE 823 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

L5 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

823

ACCESSION NUMBER: 2002:827797 CAPLUS

DOCUMENT NUMBER: 137:331022

TITLE: Coupler for azomethine dye formation and silver halide

photographic material using it

INVENTOR(S): Ogasawara, Atsushi; Kamihira, Shigeo; Shimada,

Yasuhiro PATENT ASSIGNEE(S):

Fuji Photo Film Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 28 pp.

CODEN: JKXXAF DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002318441	A	20021031	JP 2001-123651	20010420 <
PRIORITY APPLN. INFO.:			JP 2001-123651	20010420
OTHER SOURCE(S):	MARPAT	137:331022		

AB Dye forming coupler I and azomethine dye II (Q = nonmetal atoms to form N-containing heterocycle; R = substituent; Het = heterocycle; X = H, releasing group by coupling reaction with developer oxide; Ar = aryl) are claimed. The azomethine dye shows high mol. extinction coeff, clear hue, and the photog, material gives clear images with good fastness.

473738-67-9P

RL: PNU (Preparation, unclassified); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (azomethine dye; photog. coupler for azomethine dye formation)

RN 473738-67-9 CAPLUS

CN Benzoic acid, 3,3'-[[2-[[[3,4-dihydro-4-oxo-3-(phenylmethyl)-2quinazolinyl][[4-[ethyl[2-[(methylsulfonyl)amino]ethyl]amino]-2-

methylphenylliminolacetyllaminol-1H-imidazole-4,5diyl]bis(carbonylimino)]bis[4-chloro-, didodecyl ester (9CI) (CA INDEX NAME)

PAGE 2-A

- IT 473738-53-3P
 - RL: PNU (Preparation, unclassified); RCT (Reactant); TEM (Technical or engineered material use); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
- (photog. coupler for azomethine dye formation)

0

- RN 473738-53-3 CAPLUS

- RN 473738-63-5 CAPLUS CN 4H-1,2,4-Benzothiadiazine-3-acetamide,
 - a-(4,4-dimethyl-2,5-dioxo-l-imidazolidinyl)-N-(4,5-dimethyl-1Himidazol-2-yl)-4-dodecyl-, 1,1-dioxide (CA INDEX NAME)

- RN 473'38-75-9 CAPLUS

 Enzoic acid, 3,3'-[[2-[[bromo[3,4-dihydro-4-oxo-3-(phenylmethyl)-2-quinazolinyl]acetyl]amino]-Hi-mindazole-4,5-diyl]bis(carbonylimino)]bis[4-chloro-, didodecyl ester (9CI) (CA INDEX NAME)

ANSWER 6 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN 1998:682235 CAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER: 129:302639 ORIGINAL REFERENCE NO.:

TITLE:

129:61735a,61738a Preparation of

imidazolvlaminopropylindazolvlcarbonvlaminopropionate ammonioalkyl esters and related compounds as integrin αvβ3 inhibitor prodrugs.

INVENTOR(S):

Jadhav, Prabhakar; Batt, Douglas G.; Hussain, Munir A.; Pitts, William J.; Repta, Arnold J.

Du Pont Pharmaceuticals Co., USA PATENT ASSIGNEE(S):

SOURCE:

PCT Int. Appl., 311 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

DAMENIM A	10	TOTALD.	D3.000	A DDI TOAMTON NO	DATE			
PATENT 1	NO.	KIND	DATE	APPLICATION NO.	DAIL			
WO 98439	962	A1	19981008	WO 1998-US6054	19980327 <			
W:	AU, BR, CA	, CN, CZ	Z, EE, HU,	IL, JP, KR, LT, LV,	MX, NO, NZ, PL,			
	RO, SG, SI	, SK, UF	A, VN					
RW:	AT, BE, C	, DE, DF	K, ES, FI,	FR, GB, GR, IE, IT,	LU, MC, NL, PT, SE			
AU 98678	303	A	19981022	AU 1998-67803	19980327 <			
US 6214	334	B1	20010410	US 1998-49305	19980327 <			
PRIORITY APPI	N. INFO.:			US 1997-41759P	P 19970328			
				WO 1998-US6054	W 19980327			

OTHER SOURCE(S):

MARPAT 129:302639 Title compds. [I; X1-X4 = N, C; ≥2 of X1-X4 = C; R1 = specified heterocyclylalkyl; R10 = H, amino, halo, NO2, cyano, CF3, sulfonylamino, carbamoyl, (substituted) alkyl, alkoxy, alkenyl, cycloalkyl, cycloalkylalkyl, aryl, arylalkyl, etc.; R11 = H, halo, CF3, cyano, NO2, OH, amino, (substituted) alkyl, alkoxy, aryl, aralkyl, alkoxycarbonyl, alkylcarbonyl, alkylsulfonyl, alkylaminosulfonyl; W = [C(R12)2]qCONR13, CONR13[C(R12)2]q; X = CR12R14CR12R15; WX = specified piperazinylcarbonyl(alkyl); Y = COR19; R12 = H, halo, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, alkylcarbonyl, aryl, aralkyl; R13 = H, (substituted) alkyl, cycloalkylmethyl, aralkyl; R14 = H,

alkylthioalkyl, aralkylthioalkyl, aralkoxyalkyl, alkyl, alkoxyalkyl, hydroxyalkyl, alkenyl, alkynyl, cycloalkyl, aralkyl, heteroarylalkyl, aryl, heteroaryl, etc.; R15 = H, (substituted) alkyl, alkoxyalkyl, alkylaminoalkyl, aralkylcarbonyl, aryl, heteroaryl, heteroarylalkyl, aminosulfonyl, aminosulfonylamino, etc.; R19 = O(CH2)kN+R22R23R24 Z-; Z- = specified pharmaceutically acceptable anion; R22-R24 = H, (substituted) alkyl, cyclolalkylalkyl, aryl, aralkyl, heteroaryl, heteroarylalkyl; R22R23 = (substituted) 5-7 membered heterocyclyl; R22R23R24 = (substituted) heterobicvclv1; q = 0-2; k = 2-61, were prepared I may be administered by iontophoresis for the inhibition of cell adhesion, the treatment of angiogenic disorders, inflammation, bone degradation, cancer metastasis, diabetic retinopathy, thrombosis, restenosis, macular degeneration, and other conditions mediated by cell adhesion and/or cell migration and/or angiogenesis. Thus, title compound (II; R = CH2CH2N+Me3) showed electrophoretic mobility = 3.2 cm2/V/s at pH 4.5, vs. 1.7 cm2/V/s for II (R = Me).

T 185561-98-2DP, esters with ammonioalkanols

RN CN RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of imidazolylaminopropylindazolylcarbonylaminopropionate ammonioalkyl esters and related compds. as integrin inhibitor prodrugs) 185561-98-2 CAPLUS

Alanine, 3-[[[3-[4-[(4,5-dimethyl-1H-imidazol-2-yl)amino]-4-oxobutyl]-4,5-dihydro-5-isoxazolyl]carbonyl]amino]-N-[(2,4,6-trimethylphenyl)sulfonyl]-(CA INDEX NAME)

PAGE 1-A

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:76956 CAPLUS

DOCUMENT NUMBER: 126:89390

ORIGINAL REFERENCE NO.: 126:17263a,17266a

TITLE: Preparation of cyclic amides as herbicides

INVENTOR(S): Takabe, Fumiaki; Ichinohe, Yuki; Shibavama, Atsushi;

Yamaguchi, Mikio; Yanagisawa, Katsutada; Ogawa,

Yasunori; Sadohara, Hideo

PATENT ASSIGNEE(S): Kumiai Chemical Industry Co, Japan; Ihara Chemical Ind

SOURCE: Jpn. Kokai Tokkyo Koho, 37 pp.

CODEN: JKXXAF DOCUMENT TYPE: Patent LANGUAGE . Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO. DATE
JP 08311026	A	19961126	JP 1996-69068 19960229 <
JP 3954127	B2	20070808	
JP 2007182456	A	20070719	JP 2007-86387 20070329
PRIORITY APPLN. INFO.:			JP 1995-81967 A 19950314
			JP 1996-69068 A3 19960229
OTHER SOURCE(S):	MARPAT	126:89390	

AR The title compds. I [AB = NNMe, etc.; X = H, halo, etc.; m = 1 or 2; n = 1 - 3; R1 = carbamoyl with substituent, etc.] are prepared The title compound II (at 10 g) gave ≥ 90% control of Monochoria vaginalis and Scirpus juncoides.

185693-68-9P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of cyclic amides as herbicides)

RN 185693-68-9 CAPLUS

CN 1H-Pyrrole-1-acetamide, N-(4,5-dicyano-1H-imidazol-2-y1)-2,5-dihydroα,α,4-trimethyl-2-oxo-3-phenyl- (CA INDEX NAME)

L5 ANSWER 8 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:69816 CAPLUS DOCUMENT NUMBER: 126:89360

ORIGINAL REFERENCE NO.: 126:17255a,17258a

TITLE: Preparation of [(isoxazolinylalkanoyl)amino]alkanoates

and analogs as integrin antagonists INVENTOR(S):

Voss, Matthew Ernst; Jadhav, Prabhakar Kondaji; Smallheer, Joanne Marie; Batt, Douglas Guy; Pitts, William John; Wityak, John

PATENT ASSIGNEE(S): Du Pont Merck Pharmaceutical Company, USA SOURCE: PCT Int. Appl., 331 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA'	PATENT NO.					KIND DATE				APPLICATION NO.					DATE			
WO	9637	492			A1	_	1996	1128		WO 1	996-	US76	46		1	9960	524	<
	W:						BY,											
							LT,			MD,	MX,	NO,	ΝZ,	PL,	PT,	RO,	RU,	
							TM,											
							ES,											
US	5710	159			A		1998	0120		US 1	996-	6471	32		1	9960	509	<
CA	2221	980			A1		1996	1128		CA 1	996-	2221	980		1	9960	524	<
AU	AU 9658762						1996	1211		AU 1	996-	5876	2		1	9960	524	<
ZA	9604	195			A		1997	1124		ZA 1	996-	4195			1	9960	524	<
EP	8287	37							EP 1996-920476						1	9960	524	<
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,	
		IE,	FI															
JP	1150	6436			T		1999	0608		JP 1	996-	5358	99		1	9960	524	<
PRIORIT	Y APP	LN.	INFO	. :						US 1	995-	4506	46		A 1	9950	525	
										US 1	995-	4557	68		A 1	9950	531	
										US 1	996-	6471	32	- 1	A 1	9960	509	
										wo 1	996-	US 76	46	1	w 1	9960	524	
OTHER C	THED SOUDCE(S).					MADDAT 126.0026												

OTHER SOURCE(S): MARPAT 126:89360

Title compds. [(addnl.-substituted) I; R2 = Z2Z1R1; R1 = N-containing heterocyclyl; R3 = Z3ZR; R = CO2H, alkoxycarbonyl, SO3H, CONHNHSO2CF3, etc.; Z = bond (un)substituted alkylene; Z1 = bond, (0- or N-interrupted) alkylene, CO, alkanoyl (alkyl), NHCO, etc.; Z2 = bond, alkylene, phenylene, etc.; Z3 = (alkylene)carbonylimino(alkyl), etc.; dashed line = optional bond] were prepared as integrin antagonists (no data). Thus, R4(CH2)3CH:NOH (R4 = phthalimido)(preparation given) was chlorinated and the product cyclocondensed with CH2:CHCH2CO2CMe3 to give, after deprotection, tert-Bu 3-(3-aminopropyl)-2-isoxazoline-5-acetate. The latter was N-alkylated with 2-methylthio-3,4,5,6-tetrahydropyrimidine hydroiodide to give, after saponification, amidation by H2NCH2CH(NHSO2Ph)CO2Me, and saponification, title compound II.

185561-98-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of [(isoxazolinylalkanoyl)amino]alkanoates and analogs as integrin antagonists)

RN 185561-98-2 CAPLUS

CN Alanine, 3-[[[3-[4-[(4,5-dimethyl-1H-imidazol-2-yl)amino]-4-oxobutyl]-4,5dihydro-5-isoxazolyl]carbonyl]amino]-N-[(2,4,6-trimethylphenyl)sulfonyl]-(CA INDEX NAME)

PAGE 2-A

L5 ANSWER 9 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:183280 CAPLUS

DOCUMENT NUMBER: 122:55805

ORIGINAL REFERENCE NO.: 122:10814h,10815a

TITLE: A Simple and Practical Synthesis of 2-Aminoimidazoles AUTHOR(S): Little, Thomas L.; Webber, Stephen E.

Mρ

CORPORATE SOURCE: Agouron Pharmaceuticals Inc., San Diego, CA, 92121,

SOURCE: Journal of Organic Chemistry (1994), 59(24),

7299-305

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 122:55805

AB A new and simple two-step procedure to synthesize 2-aminoimidazoles (2-Al's) from readily available materials has been developed. The cyclization reaction of α -halo ketones RCOCHRIX (R = Me, Et, CMe3, Ph, 4-BrC6HH, etc., Rl = H, Me, Ph, RRl = (CH2)3, (CH2)4, X = Cl, Brl and N-acetylguanidine in acetonitrile (MeCN) at reflux, or in DMF at ambient temperature, gives 4(5)-substituted and 4/5-disubstituted N-(H+-imidazol-2-yl)acetamides I, which are then hydrolyzed to their resp. 2-Al's. In general, the purified products were isolated in good yields. We have prepared several examples and have demonstrated the usefulness of this method by its application in the total synthesis of 2-aminohistamine, an interesting histamine analog, and oroidin (II), a marine natural

product isolated from various sponges.

40639-97-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aminoimidazoles, aminohistamine, and oroidin by cyclization of carbonyl with acetylguanidine)

40639-97-2 CAPLUS RN

Acetamide, N-(4,5-dimethyl-1H-imidazol-2-yl)- (CA INDEX NAME) CN

L5 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1978:105227 CAPLUS

DOCUMENT NUMBER: 88:105227

ORIGINAL REFERENCE NO.: 88:16505a,16508a TITLE:

Thiocarbonvl vlides of 1.3-diazacvclopentadiene and of cyclopentadiene

AUTHOR(S): Gronski, Peter; Hartke, Klaus

CORPORATE SOURCE:

Inst. Pharm. Chem., Univ. Marburg, Marburg, Fed. Rep. Ger.

Chemische Berichte (1978), 111(1), 272-81 SOURCE: CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal German LANGUAGE:

OTHER SOURCE(S): CASREACT 88:105227

R1R2NCSNR3R4 (R1-R4 = H, Me; R1 = Me, R2 = R4 = H, R3 = Me, R2-R4 = H, R2R3 = CH2CH2, R4 = H, Me, R2R3 = o-C6H4, R4 = Me; R1 = R4 = H, R2R3 =

CH2CH2) reacted with imidazole I at room temperature to give 36-57% isothiuronium salts II (Z = bond) by elimination of N2. At 0°,

25-94% II (Z = N:N) were isolated as labile intermediates. Analogously, cyclopentadienide III (R5 = cyano, R6 = H) and N2NCSNH2 gave 8% isothiuronium salt IV (R1-R4, R6 = H, R5 = cyano); III (R5 = H, R6 = cyano) with R1R2NCSNR3R4 (R1 = R3 = H, R2 = R4 = Me; R1-R4 : Me; R1 = Me,

R2R3 = CH2CH2, R4 = H, Me; R1 = R4 = Me; R2R3 = o-C6H4) gave 1.5-75% IV (R5 v H, R6 = cyano). Ylides II (Z = bond) and IV are thermally stable

and are betaines. 65739-60-8P

IΤ RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) 65739-60-8 CAPLUS RN

CN Acetamide, N-(4,5-dicvano-1H-imidazol-2-vl)- (CA INDEX NAME)

DOCUMENT NUMBER: 85:5638

ORIGINAL REFERENCE NO.: 85:907a,910a

TITLE: 2-Acvlamino-4,5-di-cyanoimidazoles

INVENTOR(S): Segawa, Hirozo; Aida, Kazuhiko; Takagi, Toshiaki

PATENT ASSIGNEE(S): Kyowa Gas Chemical Industry Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp. CODEN: JKXXAF

DOCUMENT TYPE: Patent
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 51004171 A 19760114 JP 1974-74630 19740629 <--

DF 510041/1 A 19/60114 JP 19/4-74650 19/40629 C-PRIORITY APPLN. INFO:: JP 1974-74630 A 19740629 AB The title imidazoles I (R1 = C1-16 alkyl, C6-14 aryl) were prepared by

reacting II with RCOCl. Thus, 3.1 g p-MeC6H4COCl in THF was refluxed with 2.6 g II and pyridine in THF 2 hr to give I (R = C6H4Me-p). Among 6 more I similarly prepared were (R given); C6H4MO2-p, CH2Cl, CMe:CH2, CH2CD+.

T 59380-96-0P 59380-97-1P 59380-98-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 59380-96-0 CAPLUS

CN Acetamide, 2-chloro-N-(4,5-dicyano-1H-imidazol-2-yl)- (CA INDEX NAME)

RN 59380-97-1 CAPLUS

CN 2-Propenamide, N-(4,5-dicyano-1H-imidazol-2-yl)-2-methyl- (CA INDEX NAME)

RN 59380-98-2 CAPLUS

CN Acetamide, N-(4,5-dicyano-1H-imidazol-2-yl)-2-phenoxy- (CA INDEX NAME)

L5 ANSWER 12 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1975:112006 CAPLUS DOCUMENT NUMBER: 82:112006

ORIGINAL REFERENCE NO.: 82:17899a,17902a

Mononuclear heterocyclic rearrangements. VI. TITLE: Conversion of 1,2,4-oxadiazoles into imidazoles

AUTHOR(S): Ruccia, M.; Vivona, N.; Cusmano, G.

CORPORATE SOURCE: Fac. Sci., Univ. Palermo, Palermo, Italy

SOURCE: Tetrahedron (1974), 30(21), 3859-64 CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 82:112006

Condensation of aminooxadiazoles with \$\beta\$-oxo ketones or esters gave β-enamino ketones, which with NaOEt in DMF rearranged to imidazole derivs. E.g., I with (MeCO)2CH2 gave II, which with NaOEt in DMF gave III. Condensation of I with PhCOCH2CO2Et gave IV and V. V was in solution equilibrium with its tautomer VI.

ΙT 40483-42-9P 40483-44-1P 55729-98-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

40483-42-9 CAPLUS RN

CN Acetamide, N-(4-acetyl-5-methyl-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)

40483-44-1 CAPLUS RN

CN Acetamide, N-(4-benzoy1-5-methy1-1H-imidazo1-2-y1)- (9CI) (CA INDEX NAME)

55729-98-1 CAPLUS RN

CN 1H-Imidazole-4-carboxvlic acid, 2-(acetvlamino)-5-methyl-, ethyl ester (9CI) (CA INDEX NAME)

ACCESSION NUMBER: 1973:405297 CAPLUS

DOCUMENT NUMBER: 79:5297
ORIGINAL REFERENCE NO.: 79:898h,899a

TITLE: Condensations with N,N'-hydrazinodicarboxamidine. 12.

Proof of the 2-aminoimidazole structure by ring

synthesis from cyanamide
AUTHOR(S): Kreutzberger, A.; Schuecker, R.

CORPORATE SOURCE: Inst. Pharm. Chem., Westfael. Wilhelms-Univ.,

Muenster, Fed. Rep. Ger.

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1973

), 306(3), 169-73

CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal LANGUAGE: German

AB The structure of the 2-aminoimidazoles [I, R = R1 = Me or RR1 = (CH2)4] formed by reduction of the corresponding 2,2'-azoimidazoles was supported by

their synthesis from H2NCHR1COR and H2NCN.

IT 40639-97-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 40639-97-2 CAPLUS

CN Acetamide, N-(4,5-dimethyl-1H-imidazol-2-yl)- (CA INDEX NAME)

L5 ANSWER 14 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:124496 CAPLUS DOCUMENT NUMBER: 78:124496

ORIGINAL REFERENCE NO.: 78:20003a,20006a

TITLE: Condensations with hydrazine-N,N'-dicarboxamidines.

11. 2-Aminoimidazoles by reduction of

2,2'-azoimidazoles

AUTHOR(S): Kreutzberger, A.; Schuecker, R.

CORPORATE SOURCE: Inst. Pharm. Chem., Westfael. Wilhelms-Univ.,

Muenster, Fed. Rep. Ger.

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1973

), 306(2), 139-45

CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal

LANGUAGE: German
AB The aminoimidazoles XNH2 (R

B The aminoimidazoles XNH2 (R = H or Me) and YNH2 were obtained by reduction of XN:NX or YN:Ny, resp., and were characterized by conversion into acyl derivs.

T 40639-97-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) 40639-97-2 CAPLUS

CN Acetamide, N-(4,5-dimethyl-1H-imidazol-2-yl)- (CA INDEX NAME)

L5 ANSWER 15 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1973:97567 CAPLUS DOCUMENT NUMBER: 78:97567

ORIGINAL REFERENCE NO.: 78:15659a,15662a

TITLE: Mononuclear heterocyclic rearrangements. V.

1,2,4-Oxadiazoles to imidazoles

AUTHOR(S): Ruccia, Michele; Vivona, Nicolo; Cusmano, Giuseppe

CORPORATE SOURCE: Fac. Sci., Univ. Palermo, Palermo, Italy SOURCE: Tetrahedron Letters (1972), (49), 4959-60

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 78:97567

AB Condensing 3-amino-5-methyl-1,2,4-oxadiazole or the 5-Ph analog with

MeCOCH2COMe or PhCOCH2COMe in refluxing PhMe containing p-MeC6H4S03H for 8-10 hr gave the oxadiazole enamino ketones (I; R, Rl = Me, Ph). Rearrangement of I with 1 equivalent NaOSt in DMF at 110° for 3 hr gave 60-80\$ of the

corresponding imidazoles (II). Acid hydrolysis of II gave 2-aminoimidazoles.

IT 40483-42-9P 40483-44-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and acid hydrolysis of)

RN 40483-42-9 CAPLUS

CN Acetamide, N-(4-acetyl-5-methyl-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)

RN 40483-44-1 CAPLUS

CN Acetamide, N-(4-benzoyl-5-methyl-1H-imidazol-2-yl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} ACNH & \begin{matrix} H & & O \\ & & & \\ & & & \\ N & & & \\ & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

L5 ANSWER 16 OF 16 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1926:1672 CAPLUS

DOCUMENT NUMBER: 20:1672

ORIGINAL REFERENCE NO.: 20:193g-i

TITLE: AUTHOR(S): SOURCE:

2-Amino-4,5-dimethylglyoxaline Burtles, Richard; Pyman, F. L.

Journal of the Chemical Society, Transactions (

1925), 127, 2012-8 CODEN: JCHTA3: ISSN: 0368-1645

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

2-p-Bromobenzeneazo-4,5-dimethylqlyoxaline, light brown, m. 213-4° (all m. ps. are corrected); it seems to cause irritation of the skin and swelling of the eyelids; HCl salt, orange-yellow, decomps. 135°. Reduction by Sn and HCl gives 69% of 2-amino-4,5-dimethylglyoxaline-HCl, m. 389°; carbonate, with 1H2O, m. 144°; picrate, yellow, m. 245°. The amine reacts sluggishly with HNO2 in dilute or concentrated HCl or 25% AcOH, giving no crystalline products, but the solns, give deep colors on treatment with NaOH. It gives deeply colored solns. with Na2Fe(CN)6NO and aqueous NaOH or with AmNO2 and EtoNa in EtoH. Ac derivative, m. 270°; after treating with HCl and NaNo2, it gives no color with β -C10H7ONa; it instantly decolorizes aqueous KMnO4. The NH2 derivative does not give a benzylidene derivative 2-p-Bromobenzeneazo-4(5)-methylqlyoxaline (I), yellow, m. 225-6°. 5(4)-p-Bromobenzeneazo derivative, brown, m. 238°; HCl salt, vellow needles or vellow-red prisms, m. 188°. The vield of these 2 compds. is about 47 and 12%. The constitution of I was established by its reduction by Zn and AcOH to alacreatinine; this is also obtained with SnC12 and HC1, together with about 10% of the 2-amino derivative, analyzed as the picrate, brownish yellow, m. 186-7°. 40639-97-2P, Acetamide, N-(4,5-dimethyl-2-imidazolyl)-

RL: PREP (Preparation) (preparation of)

RN 40639-97-2 CAPLUS

CN Acetamide, N-(4.5-dimethyl-1H-imidazol-2-v1)- (CA INDEX NAME)

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L6 STRUCTURE UPLOADED

=> que L6

L7 QUE L6

=> d :7

L7 HAS NO ANSWERS

L6 STR



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1 ANSWERS

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L8 1 SEA SSS FUL L6

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=> s 18
L9 0 L8
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L2 QUE L1 L3 22 S L2 SSS FULL

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L4 22 S L3 L5 16 S L4 AND PY<=2004

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L6 STRUCTURE UPLOADED
L7 QUE L6
L8 1 S L7 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:40:57 ON 27 OCT 2008

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S SCRSTR/Q/REG S (L3 NOT L4)/REG

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These searches are not supported:
  S L5
  S SCRSTR/O
Example 2:
  => ACT SCRSTR2/Q
  L7
                  SCR 2127
  L8
                  OUE L6
  L9
                  OUE L7
  L10
                  QUE L8 NOT L9
  This search is supported:
  S (L6 NOT L7)/REG
  These searches are not supported:
  S L10
  S L10/REG
  S SCRSTR2/Q
  S SCRSTR2/Q/REG
  S L8 NOT L9
  S (L8 NOT L9)/REG
=> s 18
L10
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L11 STRUCTURE UPLOADED

=> que L11

L12 QUE L11

=> d 112

L12 HAS NO ANSWERS L11 STR

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126 ANSWERS

=> s 112 sss full

FULL SEARCH INITIATED 11:42:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 5244 TO ITERATE

100.0% PROCESSED 5244 ITERATIONS

SEARCH TIME: 00.00.01

L13 126 SEA SSS FUL L11

=> file caplus

COST IN U.S. DOLLARS
SINCE FILE
ENTRY
FULL ESTIMATED COST
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)
SINCE FILE
TOTAL
TOTAL

ENTRY SESSION
CA SUBSCRIBER PRICE 0.00 -12.80

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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18 FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

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=> s 113

L16

L14 44 L13

=> s 114 and py<=2004 25113423 PY<=2004

1.15 24 L14 AND PY<=2004

=> s 115 and 5-hydroxytryptamine 6834776 5

20870 HYDROXYTRYPTAMINE

71 HYDROXYTRYPTAMINES 20895 HYDROXYTRYPTAMINE

(HYDROXYTRYPTAMINE OR HYDROXYTRYPTAMINES)

20023 5-HYDROXYTRYPTAMINE (5(W) HYDROXYTRYPTAMINE)

0 L15 AND 5-HYDROXYTRYPTAMINE

=> s 115 and 5HT 3174 5HT

0 L15 AND 5HT

=> s 115 1-24 ibib ab hitstr MISSING OPERATOR L15 1-24

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s 115 1-24 ibib ab hitstr MISSING OPERATOR L15 1-24

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> file caplus COST IN U.S. DOLLARS FULL ESTIMATED COST ENTRY SESSION 9.92 643.17

FILE 'CAPLUS' ENTERED AT 11:44:31 ON 27 OCT 2008
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FILE COVERS 1907 - 27 Oct 2008 VOL 149 ISS 18 FILE LAST UPDATED: 26 Oct 2008 (20081026/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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=> d his

(FILE 'HOME' ENTERED AT 11:30:00 ON 27 OCT 2008)

FILE 'REGISTRY' ENTERED AT 11:30:38 ON 27 OCT 2008

STRUCTURE UPLOADED

L1 STRUCTURE U L2 OUE L1

L3 22 S L2 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:31:05 ON 27 OCT 2008

L5 16 S L4 AND PY<=2004

FILE 'REGISTRY' ENTERED AT 11:40:27 ON 27 OCT 2008

L6 STRUCTURE UPLOADED

L7 QUE L6 L8 1 S L7 SSS FULL

FILE 'CAPLUS' ENTERED AT 11:40:57 ON 27 OCT 2008

L9 0 S L8 L10 0 S L8

FILE 'REGISTRY' ENTERED AT 11:42:15 ON 27 OCT 2008

L11 STRUCTURE UPLOADED L12 QUE L11

L12 QUE L11 L13 126 S L12 SSS FULL

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L14
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L15
            24 S L14 AND PY<=2004
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L16 0 S L15 AND 5-HYDROXYTRYPTAMINE

L17 0 S L15 AND 5HT

FILE 'CAPLUS' ENTERED AT 11:44:31 ON 27 OCT 2008

=> s 115 1-24 ibib ab hitstr

MISSING OPERATOR L15 1-24

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> d 115 1-24 ibib ab hitstr

L15 ANSWER 1 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:80450 CAPLUS

DOCUMENT NUMBER: 140:145835

TITLE: Preparation of dibenzofused

bicyclo[2.2.2]octane-derived amides as modulators of

the glucocorticoid receptor

INVENTOR(S): Vaccaro, Wayne; Yang, Bingwei Vera; Kim, Soong-hoon; Huynh, Tram; Tortolani, David R.; Leavitt, Kenneth J.; Li, Wenying; Doweyko, Arthur M.; Chen, Xiao-tao;

Doweyko, Lidia

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA; et al.

SOURCE: PCT Int. Appl., 265 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	PATENT NO.								APPLICATION NO.								
	2004	0090	17		A2 20040129 A3 20040708										0030	717 <	
	W:	CO, GM, LS, PG,	CR, HR, LT, PH,	CU, HU, LU, PL,	CZ, ID, LV, PT,	DE, IL, MA, RO,	DK, IN, MD, RU,	AZ, DM, IS, MG, SC,	DZ, JP, MK, SD,	EC, KE, MN, SE,	EE, KG, MW, SG,	ES, KP, MX, SK,	FI, KR, MZ, SL,	GB, KZ, NI, SY,	GD, LC, NO,	GE, LK, NZ,	GH, LR, OM,
	2003	GH, KG, FI, BF, 2519	GM, KZ, FR, BJ,	KE, MD, GB, CF,	LS, RU, GR, CG, A1	MW, TJ, HU, CI,	MZ, TM, IE, CM, 2004		SL, BE, LU, GN,	SZ, BG, MC, GQ, AU 2	TZ, CH, NL, GW,	UG, CY, PT, ML, 2519	ZM, CZ, RO, MR,	ZW, DE, SE, NE,	DK, SI, SN,	EE, SK, TD, 0030	ES, TR,
EP JP	2006	273 AT, IE, 5080	BE, SI, 42	CH,	A2 DE, LV, T	DK, FI,	2005 ES, RO, 2006	0601 FR, MK, 0309	GB, CY,	GR, AL, JP 2	IT, TR, 004-	LI, BG, 5234	LU, CZ, 82	NL, EE,	SE, HU,	MC, SK	PT, 717
US							20050309			JP 2004-523482 NO 2005-74 US 2005-85347 US 2002-396877P US 2003-621909 WO 2003-US22300				20050106 20050321 P 20020718 A1 20030717			

OTHER SOURCE(S): MARPAT 140:145835

AB Title compds. I [R-R4 = H, alk(en/yn)yl, alkoxy, aryl, etc.; Z =

carboxamido, alkylamino, etc.] are prepared For instance, 2-amino-4,5-dimethylthiazole is coupled to the acid derived from the cycloaddn. of methacrylic acid and anthracene (CH3CN, EDCI, EtsN, HOAt, 18 h) to give II. I are glucocorticoid receptor modulators which are useful in treating diseases requiring glucocorticoid receptor agonist or antagonist therapy such as obesity, diabetes, inflammatory and immune disorders.

IT 650626-13-4 650626-17-8

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of dibenzofused bicyclo[2.2.2]octane-derived amides as modulators of glucocorticoid receptor)

650626-13-4 CAPLUS

CN Acetamide, N-[5-(4-fluoro-1-naphthalenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN

RN 650626-17-8 CAPLUS

CN Acetamide, N-[5-(6-methoxy-1-naphthalenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)



L15 ANSWER 2 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:80449 CAPLUS

DOCUMENT NUMBER: 140:157927

TITLE: Homology modeling of nuclear hormone receptor Site II

and design of Site II ligands
INVENTOR(S): Doweyko, Arthur; Nadler, Steven G.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 276 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

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A2 20040129 WO 2003-US22299 20030717 <--
    WO 2004009016
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
            PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
            TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
            FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
            BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
    EP 1575502
                         A2
                            20050921
                                          EP 2003-765637
                                                                 20030717
    EP 1575502
                         A3
                              20051123
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
    US 20060223110
                               20061005
                                          US 2003-621807
                        A1
                                                                20030717
PRIORITY APPLN. INFO.:
                                           US 2002-396907P
                                                             P 20020718
```

AB A binding site in nuclear hormone receptors is described and its structural coordinates are provided. The invention provides machine-readable data storage media comprising structure coordinates of Site II and computer systems comprising the machine-readable data storage media. The invention provides methods used in the design and identification of ligands of Site II and of modulators of nuclear hormone receptors. The invention provides ligands of Site II, modulators of NHRs, pharmaceutical compns. comprising modulators of NHRs, methods of modulators of an NHR. Also provided are methods of designing mutants, mutant NHRS, Site II binding assays, and models of Site II.

IT 650626-13-4P 650626-17-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(homol. modeling of nuclear hormone receptor Site II in ligand binding domain and design of Site II ligands)

RN 650626-13-4 CAPLUS

CN Acetamide, N-[5-(4-fluoro-1-naphthalenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 650626-17-8 CAPLUS

N Acetamide, N-[5-(6-methoxy-1-naphthalenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

NHAc OMe

L15 ANSWER 3 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:41450 CAPLUS

DOCUMENT NUMBER: 140:87668

TITLE: Therapeutic imidazole compounds, and human cellular

proteins casein kinase I α , δ , and

ε as targets for medical intervention against

hepatitis C virus infection Salassidis, Konstadinos; Kurtenbach, Alexander; Daub, INVENTOR(S): Henrik; Obert, Sabine

PATENT ASSIGNEE(S):

Axxima Pharmaceuticals A.-G., Germany; Greff, Zoltan; Keri, Gyoergy; Oerfi, Laszlo; Waczek, Frigyes

SOURCE: PCT Int. Appl., 89 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.					KIND DATE											
WO	2004	0052	64		A2 20040115 A3 20040304									20030707 <			
	W:	co,	CR,	CU,	CZ,	DE,	AU, DK, IN,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
		LS, PG,	LT, PH,	LU, PL,	LV, PT,	MA, RO,	MD, RU,	MG, SC,	MK, SD,	MN, SE,	MW, SG,	MX, SK,	MZ, SL,	NI, SY,	NO,	NZ,	OM,
	RW:	GH,	GM,	KE,	LS,	MW,	US, MZ, TM,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,			
		FI,	FR,	GB,	GR,	HU,	IE, CM,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
AU	2003	2499	77		A1		2004	0123		AU 2	003-	2499	77		2	0030	707 <
EP	1532	118			A2		2005	0525		EP 2	003-	7626	49		2	0030	707
	R:						ES,										PT,
US	2005						RO, 2005										105
PRIORIT	PRIORITY APPLN. INFO.:									EP 2							

OTHER SOURCE(S): MARPAT 140:87668

The invention describes imidazole compds, which are particularly useful against Hepatitis C Virus infections and diseases associated therewith. Furthermore, the invention relates to the human cellular proteins casein kinase I α , δ , and ϵ as targets for medical

intervention against Hepatitis C Virus (HCV) infections and diseases. In addition, the invention refers to a method for the identification of compds. which are useful for the prophylaxis and/or treatment of infections and diseases caused by Hepatitis C Virus, methods for treating Hepatitis C Virus infections and diseases, as well as pharmaceutical compns. useful

for the prophylaxis and/or treatment of Hepatitis C Virus infections and diseases. Moreover, the invention discloses antibodies, oligonucleotides, and specific compds. which are effective for the detection, prophylaxis and/or treatment of infections and diseases caused by Hepatitis C Virus. In addition, the invention describes solid supports useful for the identification of compds. suitable for preventing and/or treating infections and diseases caused by Hepatitis C Virus.

IT 643750-56-5

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(therapeutic imidazole compds., and human cellular casein kinase I α , δ , and ϵ as targets for medical intervention against hepatitis C virus infection)

RN 643750-56-5 CAPLUS CN Acetamide, N-14-(4-)

Acetamide, N-[4-(4-chlorophenyl)-5-(4-pyridinyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

L15 ANSWER 4 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:511143 CAPLUS

DOCUMENT NUMBER: 139:85387

TITLE: Preparation of heterocyclic substituted

phenylsulfonamides as broad-spectrum HIV protease inhibitors
INVENTOR(S): Vendeville, Sandrine Marie Helene; Verschueren, W

INVENTOR(S): Vendeville, Sandrine Marie Helene; Verschueren, Wim Gaston; Tahri, Abdellah; Moors, Samuel Leo Christiaan; Erra Sola, Montserrat

PATENT ASSIGNEE(S): Tibotec Pharmaceuticals Ltd., Ire.

SOURCE: PCT Int. Appl., 74 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	TENT		KIND DATE			APPLICATION NO.						DATE					
WO	2003	0534			A1	-	2003	0703		WO 2	002-	EP14	839		2	0021	220 <
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,
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		GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,
		LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
		PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	TJ,	TM,	TN,	TR,	TT,	TZ,
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		FΙ,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	SI,	SK,	TR,	BF,	BJ,
		CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG		
CA	2470	964			A1		2003	0703		CA 2	002-	2470	964		2	0021	220 <

AU	2002361235	A1	20030709	AU 2002-361235	200	21220 <
AU	2002361235	B2	20080724			
EP	1463502	A1	20041006	EP 2002-796754	200	21220 <
	R: AT, BE, 0	CH, DE, D	OK, ES, FR,	GB, GR, IT, LI, LU,	NL, SE, M	MC, PT,
	IE, SI, I	LT, LV, E	FI, RO, MK,	CY, AL, TR, BG, CZ,	EE, SK	
BR	2002015260	A	20041207	BR 2002-15260	200	21220 <
JP	2005513102	T	20050512	JP 2003-554192	200	21220
CN	1620292	A	20050525	CN 2002-828166	200	21220
HU	2005000164	A2	20050530	HU 2005-164	200	21220
MX	2004PA06201	A	20041206	MX 2004-PA6201	200	40621 <
NZ	533665	A	20051028	NZ 2004-533665	200	40621
IN	2004DN01777	A	20050401	IN 2004-DN1777	200	40622
NO	2004003114	A	20040920	NO 2004-3114	200	40720 <
ZA	2004005784	A	20050831	ZA 2004-5784	200	40720
US	20050222215	A1	20051006	US 2005-499221	200	50412
PRIORIT	Y APPLN. INFO.	:		EP 2001-205115	A 200	11221
				WO 2002-EP14839	W 200	21220

OTHER SOURCE(S): MARPAT 139:85387

B RILN(R2)CHR3CH(OH)CH2N(R4)SO2C6H4R5 [R1 = H, alkyl, alkenyl, aralkyl, cycloalkyl, cycloalkylalkyl, aryl, heterocyclic, heterocyclylalkyl, (un)substituted CH2CH2NH2; L = CO, O2C, (un)substituted NHCO,

oxaalkylcarbonyl, aminoalkylcarbonyl, 502, 035, (un)substituted NHSO2; R2 = H, alkyl; R3 = alkyl, aryl, cycloalkyl, cycloalkylalkyl, aralkyl; R4 = H, (un)substituted CO2H, COMH2, cycloalkyl, alkenyl, alkynyl, alkyl; R5 = (un)substituted heteroaryl] were prepared for use as broad-spectrum HIV protease inhibitors. Thus, (1S, 2R)-Me3CO2CNHCH(CH2Ph)CH(OH)CH2NHCH2CHMe2 was treated with 4-NCC6H4SO2Cl to give

(1S, 2R)-Me3CO2CNHCH(CH2Ph)CH(OH)CH2N(CH2CHMe2)SO2C6H4CN-4 which was deblocked and treated with the

hexahydrofurofuranyloxycarbonyloxypyrrolidinedione to give the carbamate I [R6 = CN]. Treatment of I [R6 = CN] with NH2OH.HCl gave I [R6 = CNH2):NOH] which was cyclized with 2-furoyl chloride to give I [R6 = 5-(2-furyl)-1,2,4-oxadiazol-3-yl] which had pEC50 = 8.4 for inhibition of HIV-1.

IT 553644-43-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic substituted phenylsulfonamides as broad-spectrum HIV protease inhibitors)

RN 553644-43-2 CAPLUS

CN Carbamic acid, [(15,2R)-3-[[[4-[2-(acetylamino)-1H-imidazol-4-yl]phenyl]sulfonyl](2-methylpropyl)amino]-2-hydroxy-1-(phenylmethyl)propyl]-, (3R,3aS,6aR)-hexahydrofuro[2,3-b]furan-3-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

- 553645-06-0P 553645-07-1P
 - RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of heterocyclic substituted phenylsulfonamides as broad-spectrum HIV protease inhibitors)

- 553645-06-0 CAPLUS RN
- Acetamide, N-[5-[4-[[[(2R,3S)-3-[bis(phenylmethyl)amino]-2-hydroxy-4phenylbutyl](2-methylpropyl)amino]sulfonyl]phenyl]-1H-imidazol-2-yl]- (CA INDEX NAME)

Absolute stereochemistry.

- 553645-07-1 CAPLUS
- Acetamide, N-[5-[4-[[(2R,3S)-3-amino-2-hydroxy-4-phenylbuty1](2methylpropyl)amino]sulfonyl]phenyl]-1H-imidazol-2-yl]- (CA INDEX NAME)

Absolute stereochemistry.

RECORD, ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 5 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:58069 CAPLUS

DOCUMENT NUMBER: 138:122639

TITLE: Preparation of thiazols and related compounds as

THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS

telomerase inhibitors INVENTOR(S): Priepke, Henning; Kauffmann-Hefner, Iris; Hauel,

Norbert; Damm, Klaus; Schnapp, Andreas

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K.-G., Germany

PCT Int. Appl., 88 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT:

REFERENCE COUNT:

PATENT INFORMATION:

PATENT NO. KIND APPLICATION NO. DATE DATE

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WO 2003006443
                       A2 20030123 WO 2002-EP7558 20020706 <--
    WO 2003006443
                       A3 20030501
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
            PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
            UA, UG, US, UZ, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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            FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF,
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                                          AU 2002-328323
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                                          US 2002-192456
    US 20030055263
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PRIORITY APPLN. INFO.:
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                                          US 2001-307449P
                                                            P 20010724
                                                            W 20020706
                                          WO 2002-EP7558
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OTHER SOURCE(S): MARPAT 138:122639

Title compds. R1-A-B-R2 (I) [R1 = (un)substituted Ph, phenylalkyl, phenylalkenyl, etc.; A = (un)substituted phenylalkyl; B = HN, NHCO, CONH, etc.; R2 = CO2, (un)substituted cycloalkyl, cycloalkenyl, etc. | and their pharmaceutically acceptable salts were prepared For example, coupling of thiazol II and phthalic anhydride afforded claimed benzoic acid III in 30% yield. In telomerase inhibition studies, 3-specific examples of I exhibited IC50 values ranging from $< 1 - < 5 \mu M$, e.g., IC50 value of compound III was < 5 µM. Compds. I are claimed useful as telomerase inhibitors.

160072-53-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of thiazols and related compds. as telomerase inhibitors)

160072-53-7 CAPLUS RN

CN Acetamide, N-[5-(2-naphthalenv1)-1H-imidazo1-2-v1]- (CA INDEX NAME)

L15 ANSWER 6 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:855867 CAPLUS

DOCUMENT NUMBER: 139:214346

TITLE:

Product class 3: imidazoles

Grimmett, M. R. AUTHOR(S):

Organic Chemistry, Dept. of Chemistry, University of CORPORATE SOURCE:

Otago, Dunedin, N. Z. SOURCE:

Science of Synthesis (2002), 12, 325-528

CODEN: SSCYJ9 Georg Thieme Verlag

PUBLISHER: DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

A review. Methods for preparing imidazoles are reviewed including AB cyclization, ring transformations, aromatization and modification of substituents on existing imidazoles.

160041-64-5P 160072-51-5P 160072-52-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of imidazoles via cyclization, ring transformation, aromatization and substituent modifications)

RN 160041-64-5 CAPLUS

CN Acetamide, N-(5-phenyl-1H-imidazol-2-yl)- (CA INDEX NAME)

RN 160072-51-5 CAPLUS

CN Acetamide, N-(4-methyl-5-phenyl-1H-imidazol-2-yl)- (CA INDEX NAME)

RN 160072-52-6 CAPLUS

CN Acetamide, N-(4,5-diphenyl-1H-imidazol-2-yl)- (CA INDEX NAME)

REFERENCE COUNT:

823 THERE ARE 823 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 7 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2002:773670 CAPLUS

DOCUMENT NUMBER: 137:279200

TITLE: Preparation of novel benzotriazoles as

anti-inflammatory compounds

INVENTOR(S): Dombroski, Mark Anthony; Laird, Ellen Ruth; Letavic,

Michael Anthony; McClure, Kim Francis

PATENT ASSIGNEE(S): Pfizer Products Inc., USA

SOURCE: Eur. Pat. Appl., 69 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	ENT	NO.			KIN	D	DATE			APPL	ICAT	ION I	NO.		D.	ATE		
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EP	1247	810			A1		2002	1009		EP 2	002-	2521	53		2	0020	326	<
EP	1247	810			В1		2005	0907										
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IE, SI, LT, LV, FI, RO, MK, CY, AL, TR AT 304009 \mathbf{T} 20050915 AT 2002-252153 20020326 ES 2247271 Т3 20060301 ES 2002-252153 20020326 CA 2379903 20021004 CA 2002-2379903 20020402 <--A1 20060801 CA 2379903 С JP 2002308872 Α 20021023 JP 2002-102969 20020404 <---JP 3832646 20061011 B2 US 20030078432 A1 20030424 US 2002-115952 20020404 <--US 6664395 B2 20031216 BR 2002001087 Α 20030527 BR 2002-1087 20020404 <--MX 2002PA03454 Α 20040716 MX 2002-PA3454 20020404 <--PRIORITY APPLN. INFO.: US 2001-281331P P 20010404

OTHER SOURCE(S): MARPAT 137:279200

The title compds. [I; Het = (un)substituted pyrrolyl, imidazolyl, pyrazolyl, oxazolyl, etc.; R2 = H, alkyl, cycloalkyl, etc.; R3 = H, alkyl, Ph, etc.; s = 0-5] which are potent inhibitors of MAP kinases, preferably p38 kinase (no data given), and are useful in the treatment of inflammation, osteoarthritis, rheumatoid arthritis, cancer, reperfusion or ischemia in stroke or heart attack, autoimmune diseases and other

disorders, were prepared Thus, treating a solution of 3-isopropv1-3H-benzotriazole-5-carbaldehydein THF with concentrate NH4OH followed by addition of piperazine and isocvanide II afforded III.

467234-98-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of novel benzotriazoles as antiinflammatory agents) RN 467234-98-6 CAPLUS

CN Acetamide, N-[5-(1-methyl-1H-benzotriazol-6-yl)-4-(3-methylphenyl)-1Himidazo1-2-v11- (CA INDEX NAME)

REFERENCE COUNT: THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 8 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN 2002:716272 CAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 137:232656

TITLE: Preparation of

5-(phenylheteroaryl)-1,3-dihydro-2-benzimidazolone MAP kinase inhibitors as anti-inflammatory agents

INVENTOR(S): Dombroski, Mark Anthony; Letavic, Michael Anthony;

McClure, Kim Francis PATENT ASSIGNEE(S):

Pfizer Products Inc., USA SOURCE: PCT Int. Appl., 272 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

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PATENT NO.
                        KIND DATE APPLICATION NO. DATE
    WO 2002072576 A1 00000
                         A1 20020919 W0 2002-IB334 20020130 <--
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,
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             CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
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     CA 2440211
                         A1
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                                                                     20020130 <--
     EP 1370557
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                          A1
     EP 1370557
                                20051116
                         B1
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
                                           BR 2002-7957
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     BR 2002007957
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                                20040902
                                                                     20020130 <--
                         T
     AT 309997
                                20051215
                                                                     20020130
    AI 309997 I 20031215
ES 2251582 T3 20060501
US 20030092749 A1 20030515
US 7056918 B2 20060606
MX 2003PA08142 A 20031212
                                                                     20020130
                                                                     20020311 <--
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                                                                     20030909 <--
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US 2001-274791P P 20010309
WO 2002-IB334 W 20020130
PRIORITY APPLN. INFO.:
                     CASREACT 137:232656; MARPAT 137:232656
OTHER SOURCE(S):
    Title compds. I [wherein Het = (un)substituted pyrrolyl, imidazolyl,
     pyrazolyl, oxazolyl, isoxazolyl, thiazolyl, or isothiazolyl; R1 and R2 =
     independently H or (un) substituted (cyclo) alkyl, Ph, heteroaryl, or
     heterocyclyl; R3 = independently halo, (perhalo)alkyl,
     (perhalo)cycloalkyl, alkenyl, alkynyl, heterocyclyl(oxy), Ph, OH,
     (perhalo)alkoxy, OPh, alkylthio, alkyl(amino)sulfonyl, alkylsulfamoyl,
     carbamoyl, acyl, carboxy, etc.; n = 0-5] were prepared as potent inhibitors
     of MAP kinases, preferably p38 kinase. For example,
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(perhalo)alkoxy, OPh, alkylthio, alkyl(amino)sulfonyl, alkylsulfamoyl, carbamoyl, acyl, carboxy, etc.; n = 0-5) were prepared as potent inhibitors of MAP kinases, preferably p38 kinases. For example, (3R)-(-)-lbenzyl-3-aminopyrrolidine was condensed with 1,3-diethyl-2-oxo-2,3-dihydro-1H-benzimidazolo-5-carbaldehyde in the presence of Mg504 in CH2Cl2. Addition of ((4-methylphenylsulfonyl)(m-tolyl)methyllisocyanide to the 5-(benzylpyrrolidinyliminomethyl)benzimidazolone using DMF and MP-carbonate gave the 5-(m-tolyl)midazolyl derivative Treatment with Pd/C and HCl in MeOH afforded (R)-II-HCl. All of the compds. of the invention that were tested had an IC50 < 10 MM in TNFa and MAPKAP

in vitro assays and an ED50 < mg/kg in an in vivo Thra assay. I are useful in the treatment of inflammation, osteoarthritis, rheumatoid arthritis, cancer, reperfusion of ischemia in stroke or heart attack, autoimmune diseases, and other disorders (no data).

IT 459184-45-3P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(anti-inflammatory agent; preparation of (phenylheteroaryl)benzimidazolone MAP kinase inhibitors as anti-inflammatory agents)

RN 459184-45-3 CAPLUS

CN Acetamide, N-[5-(3-chloropheny1)-4-(1-cyclopenty1-2,3-dihydro-3-methy1-2-oxo-1H-benzimidazo1-5-y1)-1H-imidazo1-2-y1]- (CA INDEX NAME)

1T 459183-44-9P, N-[5-(1-Isobuty1-3-methy1-2-oxo-2,3-dihydro-1H-benzimidazo1-5-y1)-4-(m-toly1)-1H-imidazo1-2-y1)acetamide 459183-59-6P 459183-75-6P 459183-83-6P 459184-04-4P 459184-13-5P 459184-21-5P 459184-03-1P 459184-53-1P 459184-53-1P 459184-53-1P 459185-1P 459185-1P 459185-17-2P 459185-25-2P 459185-32-2P 459185-17-2P 459185-25-2P 459185-33-2P 459185-41-2P 459185-25-2P 459185-31-P 459185-41-2P 459185-36-PP 459185-57-0P 459185-88-7P 459185-96-7P 459186-55-1P 459186-17-5P 459186-24-4P 459186-55-1P 459187-39-4P 819187-39-4P 819187-

(anti-inflammatory agent; preparation of (phenylheteroaryl)benzimidazolone MAP kinase inhibitors as anti-inflammatory agents)

RN 459183-44-9 CAPLUS

CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 459183-59-6 CAPLUS

CN Acetamide, N-[5-(1,3-diethyl-2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-4-(3-methylphenyl)-1H-imidazol-2-yl)- (CA INDEX NAME)

RN 459183-75-6 CAPLUS

CN Acetamide, N-[5-(2,3-dihydro-1,3-dimethyl-2-oxo-1H-benzimidazol-5-yl)-4-(4-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

- RN 459183-83-6 CAPLUS
- CN Acetamide, N-[5-(2,3-dihydro-1,3-dimethyl-2-oxo-1H-benzimidazol-5-yl)-4phenyl-1H-imidazol-2-yl]- (CA INDEX NAME)

- RN 459184-04-4 CAPLUS
- CN Acetamide, N-[5-(2,3-dihydro-1,3-dimethyl-2-oxo-1H-benzimidazol-5-yl)-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

- RN 459184-13-5 CAPLUS
- CN Acetamide, N-[5-(1,3-diethyl-2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-4-(4-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

- RN 459184-21-5 CAPLUS
- CN Acetamide, N-[5-(1,3-diethyl-2,3-dihydro-2-oxo-1H-benzimidazol-5-yl)-4-phenyl-1H-imidazol-2-yl]- (CA INDEX NAME)

- RN 459184-53-3 CAPLUS
- CN Acetamide, N-[5-(1-cyclopentyl-2,3-dihydro-3-methyl-2-oxo-1H-benzimidazol-5-yl)-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

- RN 459184-69-1 CAPLUS
- CN Acetamide, N-[5-[1-(cyclopropylmethyl)-2,3-dihydro-3-methyl-2-oxo-1H-benzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 459184-85-1 CAPLUS

CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropy1)-2-oxo-1H-benzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 459184-93-1 CAPLUS

CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 459185-01-4 CAPLUS

CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-v1]-4-(3-methylphenyl)-1H-imidazol-2-v1]- (CA INDEX NAME)

RN 459185-09-2 CAPLUS

CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazo1-5-yl]-4-(4-fluorophenyl)-1H-imidazo1-2-yl]-2-methoxy- (CA INDEX NAME)

RN 459185-17-2 CAPLUS

CN Propanamide, N-[5-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]-2-methyl- (CA INDEX NAME)

RN 459185-25-2 CAPLUS

CN Propanamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]-2-methyl- (CA INDEX NAME)

RN 459185-33-2 CAPLUS

RN 459185-41-2 CAPLUS

CN Butanamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]-3,3-dimethyl- (CA INDEX NAME)

RN 459185-49-0 CAPLUS

CN Butanamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]-3,3-dimethyl- (CA INDEX NAME)

RN 459185-57-0 CAPLUS

CN Butanamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]-3-methyl- (CA INDEX NAME)

RN 459185-88-7 CAPLUS

CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazo1-5-yl]-4-(3-methylphenyl)-1H-imidazo1-2-yl]-2-methoxy- (CA INDEX NAME)

RN 459185-96-7 CAPLUS

CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1H-benzimidacol-5-yl]-4-(3-methylphenyl)-1H-imidacol-2-yl]-2-methoxy- (CA INDEX NAME)

RN 459186-03-9 CAPLUS

CN

Butanamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-lH-benzimidazol-5-yl]-4-(3-methylphenyl)-lH-imidazol-2-yl]-3-methyl- (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Me} \\ i-Bu-C-NH & N & 0 \\ N & N & N \\ & & N \\ & & & N \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & &$$

RN 459186-17-5 CAPLUS CN Propanamide, N-[5-[2,3-dihydro-3-methyl-1-(2-methylpropyl)-2-oxo-1Hbenzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

$$\begin{array}{c} 0 \\ \text{Et-C-NH} \\ N \end{array}$$

459186-24-4 CAPLUS RN CN

Acetamide, N-[5-[2,3-dihydro-3-methyl-2-oxo-1-(tetrahydro-3-furanyl)-1Hbenzimidazol-5-yl]-4-(4-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 459186-55-1 CAPLUS

CN Acetamide, N-[5-[2,3-dihydro-3-methyl-2-oxo-1-(tetrahydro-3-furanyl)-1Hbenzimidazol-5-yl]-4-(3-methylphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 459187-09-8 CAPLUS

CN Acetamide, N-[4-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-yl]-5-(3-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 459187-16-7 CAPLUS

CN Acetamide, N-[4-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-yl]-5-(2-fluorophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 459187-24-7 CAPLUS

CN Acetamide, N-[4-(4-chlorophenyl)-5-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1H-benzimidazol-5-yl]-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 459187-39-4 CAPLUS

CN Acetamide, N-[5-[2,3-dihydro-3-methyl-1-(1-methylethyl)-2-oxo-1Hbenzimidazol-5-yl]-4-phenyl-1H-imidazol-2-yl]- (CA INDEX NAME)

REFERENCE COUNT: THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 9 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:

DOCUMENT NUMBER: 134:311218

2001:283949 CAPLUS TITLE: Synthesis and use of heterocyclic sodium/proton

exchange inhibitors INVENTOR(S):

Ahmad, Saleem; Wu, Shung C.; O'Neil, Steven V.; Ngu, Khehyong; Atwal, Karnail S.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

A1

SOURCE: PCT Int. Appl., 221 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

CA 2388813

KIND APPLICATION NO. PATENT NO. DATE DATE --------------_____ WO 2001027107 A2 20010419 WO 2000-US27461 20001002 <--WO 2001027107 A3 20020124 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG US 6887870 B1 20050503 US 2000-669298 20000925

CA 2000-2388813

20001002 <--

20010419

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MX	2002PA03626	5 A	20030922	MX 2002-PA3626	20020410 <
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PRIORITY	APPLN. IN	FO.:		US 1999-158755P	P 19991012
				US 2000-669298	A3 20000925
				WO 2000-US27461	W 20001002

OTHER SOURCE(S): MARPAT 134:311218

Compds. of formula I [wherein; n is 1-5; X is N or CR5, where R5 is H, halo, alkenyl, alkynyl, alkoxy, alkyl, aryl or heteroaryl; Z is a heteroaryl group; R1 is H, alk(en)(yn)yl, alk(enyl)(ynyl)oxy, (aryl or alkyl)3Si, cycloalk(en)yl, (aryl)amino, aryl(alkyl), cycloheteroaryl, etc.; R2, R3 and R4 are any of the groups set out for R1 and optionally substituted with 1 to 5 substituents which may be the same or different and when X is N, R1 is preferably aryl or heteroaryl] are claimed. Several hundred examples are disclosed. Synthesis of II proceeds via cyclopropanation of the cinnamate derived from the olefination between 3,5-dichlorobenzaldehyde and t-butyldiethylphosphonoacetate. The intermediate tert-Bu ester is converted to the corresponding α-chloroketone and reacted with acetyl quanidine to provide II in a total of 5 steps. Compds. I are said to be sodium/proton exchange inhibitors (NHE). Pharmaceutical combinations are claimed using I and certain antihypertensive agents, β -adrenergic agonists, hypolipidemic agents, antidiabetic agents, antiobesity agents, etc. Compds. I are useful as antianginal and cardioprotective agents and provide a method for preventing or treating angina pectoris, cardiac dysfunction, myocardial necrosis, and arrhythmia.

IT 335061-48-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (synthesis and use of heterocyclic sodium/proton exchange inhibitors)

RN 335061-48-8 CAPLUS CN Acetamide, N-14-1(1R

Acetamide, N-[4-[(1R,3R)-3-(3-chlorophenyl)-2,2-dimethylcyclopropyl]-5phenyl-1H-imidazol-2-yl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

L15 ANSWER 10 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2000:98527 CAPLUS

DOCUMENT NUMBER: 132:137388

TITLE: Preparation of N-imidazolvlalkvl-2-imidazoleamines as

histamine H3 receptor ligands INVENTOR(S): Jegham, Samir; Saady, Mourad; Yaiche, Philippe;

French

Horter, Laurence PATENT ASSIGNEE(S):

Sanofi-Synthelabo, Fr.

SOURCE: PCT Int. Appl., 23 pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent.

LANGUAGE: FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

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PA	TENT				KIN	D	DATE			APPL.	ICAT.	TON .	NO.				
						_											
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		JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,
		MN,	MW,	MX,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,
		TM,	TR,	TT,	UA,	UG,	US,	UΖ,	VN,	YU,	ZA,	ZW,	AM,	ΑZ,	BY,	KG,	KZ,
		MD,	RU,	TJ,	TM												
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		CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG					
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FR	2781	798			B1		2000	0908									
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PRIORIT	Y APP	LN.	INFO	. :						FR 1	998-	9602			A 1	9980	728
										WO 1	999-1	FR18	24		W 1	9990	726

OTHER SOURCE(S): MARPAT 132:137388

RZNH(CH2)mR1 (R1 = 1H-imidazole-4-yl)[I; R = (un)substituted Ph; Z = (un) substituted 1H-imidazole-5, 2-diyl; m = 2-4] were prepared Thus, PhCH(OH)COPh was cyclocondensed with urea and the chlorinated product

aminated by H2CH2Ph to give, after deprotection,

4,5-diphenyl-1H-imidazole-2-amine which was amidated by 1H-imidazole-4-propanoic acid and the product reduced to give I (R = Ph, Z = 3-phenvl-1H-imidazole-5,2-divl, m = 3). Data for biol. activity of I were given.

256657-13-3P 256657-15-5P 256657-16-6P

256657-18-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-imidazolvlalkyl-2-imidazoleamines as histamine H3 receptor ligands)

256657-13-3 CAPLUS RN

1H-Imidazole-5-propanamide, N-(4,5-diphenyl-1H-imidazol-2-yl)-, CN hydrochloride (1:2) (CA INDEX NAME)

●2 HC1

RN 256657-15-5 CAPLUS

CN

1H-Imidazole-5-propanamide, N-[5-(4-fluoropheny1)-1H-imidazol-2-y1]- (CA INDEX NAME)

256657-16-6 CAPLUS

CN 1H-Imidazole-5-propanamide, N-[5-(4-chloro-3-methylphenyl)-1H-imidazol-2vl]- (CA INDEX NAME)

RN 256657-18-8 CAPLUS

CN 1H-Imidazole-5-butanamide, N-(5-phenyl-1H-imidazol-2-yl)- (CA INDEX NAME)

$$(CH_2)_3 - C - NH \longrightarrow Ph$$

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 4 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 11 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:723017 CAPLUS

DOCUMENT NUMBER: 131:337034

TITLE: Preparation of 1-naphthylsulfonyl-4-heteroarylbenzoylpiperazines and

analogs as Factor Xa inhibitors

INVENTOR(S): Nowak, Thorsten; Preston, John; Rayner, John Wall;

Smithers, Michael James; Stocker, Andrew PATENT ASSIGNEE(S): Zeneca Limited, UK

SOURCE: PCT Int. Appl., 39 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

		CENT :																	
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	WO	9957	099			A1		1999	1111		WO 1	999-0	GB13	12		1	9990	427	<
		W:	AE,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	
			DE.	DK.	EE,	ES.	FI.	GB,	GD,	GE,	GH.	GM.	HR.	HU.	ID.	IL.	IN.	IS,	
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		1082									EF I	JJJ-	2101	15		1	JJJ0	42/	
	EF										0.5	T.m.				0.77			
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		2878																	
		6395				BI		2002	0528										<
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											WO 1	999-1	GB13	12	1	W 1	9990	427	
OTHER																			
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	(ur	ı) sub	stit	uted	by :	1-3 1	nalo	, ox	o, C	Э2Η,	CF3	, CN	, NH:	2, 0	H, No	02,			
	(ar	nino)	alky	1, a	lkox	y (car	cbon	y1),	and	/or	(di)	alky.	lami	no;	Y =	(un)	subs	titu	ted
	phe	envle	ne;	z =	(un)	subst	itu	ited 1	oipe:	ridi	ne-4	. 1-d	ivl	or p	iper	azin	e-1.	4-di	vl:
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µM for thrombin inhibition (no individual data given). Data for anticoagulant activity of I in conventional prothrombin time tests were given.

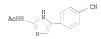
IT 249887-81-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of 1-naphthylsulfonyl-4heteroarylbenzoylpiperazines and analogs as Factor Xa inhibitors for treatment of thrombosis mediated diseases and coagulation disorders) 249887-81-8 CAPLUS

CN Acetamide, N-[5-(4-cyanophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

1-(6-chloronaphth-2-ylsulfonyl)piperazine to yield the title imidazolylbenzoylpiperazine (II). The IC50 values of invention compds. ranged from 0.001 to 0.1 µM for Factor Xa inhibition and were > 40



REFERENCE COUNT:

RN

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

10

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DOCUMENT NUMBER:
                        131:271809
TITLE:
                        Preparation of
```

3-(α-heteroarylaminobenzylidene)-2-indolinones

as Cyclin dependent kinase inhibitors

Grell, Wolfgang; Walter, Rainer; Heckel, Armin; INVENTOR(S): Himmelsbach, Frank; Wittneben, Helmut; van Meel, Jakobus; Redemann, Norbert; Haigh, Robert

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma K .- G., Germany SOURCE: Ger. Offen., 64 pp.

CODEN: GWXXBX DOCUMENT TYPE: Patent German

LANGUAGE: FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

	TENT						DATE				ICAT					ATE		
	1981						1999	1007								9980	403 ·	<
US	6043	254			A		2000	0328		US 1	999-	2770	63		1	9990	326 -	<
WC	9951	590			A1		1999	1014		WO 1	999-	EP21	86		1	9990	330 -	<
	W:	AE.	AL.	AM.	AT.	AU.	AZ,	BA.	BB.	BG.	BR.	BY.	CA.	CH.	CN.	CU.	CZ.	
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							ML,						JE,	DE,	ы,	CF,	co,	
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					А		1999	1025										
PRIORIT	Y APP	LN.	TNEO	. :							998-							
											998-				P 1			
										WO 1	999-	EP21	86		W 1	9990	330	
OTHER S																		
AB Ti	AB Title compds. [I; R = H; R1 = H, halo, NO2, (alkanoyl)amino, etc.; R2 =																	
(u	n) sub	stit	uted	Ph;	R4 :	NH	IR3;	R3 =	het	eroa	nnel	ated	Ph,					
le e		7 -	11. / -	- V T	-1	- 7		3				TP 1	- 0	1 - 1 -	1 4			

heteroarylalk(en)ylphenyl, etc.] were prepared Thus, 2-indolinone was N-acetylated and the product condensed with PhC(OEt)3 to give I (R1 = H,

R2 = Ph)(II; R = Ac, R4 = OEt) which was condensed with 5-aminoindole to give II (R = H, R4 = 5-indolvlamino). Data for biol. activity of I were given.

245546-35-4P 245546-36-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of 3-(α-heteroarylaminobenzylidene)-2-indolinones as

cyclin dependent kinase inhibitors)

245546-35-4 CAPLUS RN CM

Acetamide, N-[5-[4-[[(Z)-(1,2-dihydro-5-nitro-2-oxo-3H-indol-3ylidene)phenylmethyl]amino]phenyl]-1H-imidazol-2-yl]- (CA INDEX NAME)

Double bond geometry as shown.

RN 245546-36-5 CAPLUS

CN Acetamide, N-[5-[4-[[(Z)-(1,2-dihydro-5-nitro-2-oxo-3H-indol-3-ylidene)phenylmethyl]amino]phenyl]-4-methyl-1H-imidazol-2-yl]- (CA INDEX NAME)

Double bond geometry as shown.

IT 96139-64-9P 96139-70-7P 160072-51-5P

245546-86-5P 245546-87-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 3-(α -heteroarylaminobenzylidene)-2-indolinones as cyclin dependent kinase inhibitors)

RN 96139-64-9 CAPLUS

CN Acetamide, N-[5-(4-aminophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 96139-70-7 CAPLUS

CN Acetamide, N-[5-(4-nitrophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 160072-51-5 CAPLUS

CN Acetamide, N-(4-methy1-5-pheny1-1H-imidazo1-2-y1)- (CA INDEX NAME)

RN 245546-86-5 CAPLUS

CN Acetamide, N-[4-methyl-5-(4-nitrophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 245546-87-6 CAPLUS

CN Acetamide, N-[5-(4-aminophenyl)-4-methyl-1H-imidazol-2-yl]- (CA INDEX NAME)

L15 ANSWER 13 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:109589 CAPLUS

DOCUMENT NUMBER: 130:237506

TITLE: Synthesis of novel 4,5-diphenylthiazole derivatives as potential acyl-CoA: cholesterol O-acyltransferase

inhibitors

AUTHOR(S): Romeo, G.; Salerno, L.; Milla, P.; Siracusa, M.;

Cattel, L.; Russo, Filippo
Dip. Scienze Farmaceutiche, Univ. Catania, Catania,

CORPORATE SOURCE: Dip. Scienze F. I-95125, Italy

SOURCE: Pharmazie (1999), 54(1), 19-23 CODEN: PHARAT; ISSN: 0031-7144

PUBLISHER: Govi-Verlag Pharmazeutischer Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 130:237506

AB Several N-(4,5-diphenylthiazol-2-yl)-N-aryl- or -alkyl-(thio)ureas and N-(4,5-diphenylthiazol-2-yl)alkanamides were prepared as potential acyl-CoA: cholesterol O-acyltransferase (ACAT) inhibitors. Synthesis was accomplished by reaction of 2-amino-4,5-diphenylthiazole with suitable isocyanates, isothiocyanates, or acyl chlorides. Some analogs without a 5-Ph substituent or both the Ph groups in 4- and 5-position of the thiazole ring were also prepared Moreover, some bio-isosteres of the title

compds. in which the thiazole ring was replaced by an imidazole were synthesized starting from 2-amino-4,5-diphenyl-lH-imidazole. The ability of synthesized compds. to inhibit ACAT was evaluated in vitro by measuring the formation of cholesteryl[14C]oleate from cholesterol and [1-14C]oleath formation of rat liver microsomes. Among the tested compds., only some thiazole ureas were able to inhibit ACAT in a reasonable degree. N-(4,5-diphenylthiazol-2-yl)-N'-[2,6-bis(2-methylethyl)phenyllyrea and N-(4,5-diphenylthiazol-2-yl)-N'-butylurea were the most active compds. in the series showing ICSO values in the low micromolar range. 221389-49-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of phenylthiazoles cholesterol O-acyltransferase inhibitors)
RN 221389-49-7 CAPLUS

CN Hexanamide, N-(4,5-diphenyl-1H-imidazol-2-yl)- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 14 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:217660 CAPLUS

DOCUMENT NUMBER: 128:277027

ORIGINAL REFERENCE NO.: 128:54715a,54718a

TITLE: Silver halide photographic material and its processing method providing superior silver tone

INVENTOR(S): Yamashita, Hiroshi PATENT ASSIGNEE(S): Konica Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 33 pp. CODEN: JKXXAF

DOCUMENT TYPE: Patent
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10090821 PRIORITY APPLN. INFO.:	A	19980410	JP 1996-244931 JP 1996-244931	19960917 <
			OF 1330-244331	13300317
OTHER SOURCE(S):	MARPAT	128:277027		

B The material comprises ≥1 Ag halide emulsion layer on ≥1 side of a support and ≥1 hydrophilic colloid layer containing a leuco dye producing blue color in reaction with an oxidized developer and a branched cyclodextrin and/or a cyclodextrin polymer. The material is processed with a developer containing ascorbic acid-type compound Q1C(:Q3)CR1:CR2Q2 (I; R1, R2 = OH, amino, acylamino, alkylsulfonylamino, arylsulfonylamino, alkoxycarbonylamino, mercapto, alkylthic; Q1, Q2 = OH, CO2H, alkoxy, hydroxyalkyl, carboxyalkyl, sulfo, sulfoalkyl, amino, aminoalkyl, alkyl, aryl, non-metallic atoms required to form a 5- to 8-membered ring with a carbon substituted with R1, R2, and Q3; Q3 = O, NR3; R3 = H, OH, alkyl, acyl, hydroxyalkyl, sulfoalkyl, carboxyalkyl) and an auxiliary developer. Alternatively, the material without the

cyclodextrin-based component is processed with a developer containing I, an auxiliary developer, a branched cyclodextrin and/or a cyclodextrin polymer. The material processed by the method shows superior silver tone and stable photog, properties even in running processing with lower replenishment of an ascorbic acid and its derivative instead of a hydroguinone.

IT 205577-10-2

CN

RL: MOA (Modifier or additive use); USES (Uses)

(leuco dye; silver halide emulsion containing blue-color-forming leuco dye reactive to oxidized photog. developer)

RN 205577-10-2 CAPLUS

Propanamide, N-[4-[2-(acetylamino)phenyl]-5-[[4-(diethylamino)-2-methylphenyl]amino]-1H-imidazol-2-yl]-2,2-dimethyl- (CA INDEX NAME)

L15 ANSWER 15 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:472632 CAPLUS

DOCUMENT NUMBER: 125:127626
ORIGINAL REFERENCE NO.: 125:23665a,23668a

ORIGINAL REFERENCE NO.: 125:23665a,23668a
TITLE: Silver halide photo

TITLE: Silver halide photographic material containing anilinoimidazole to develop dye image with high

spectral absorption

INVENTOR(S): Ookawa, Atsuhiro; Sakai, Minoru PATENT ASSIGNEE(S): Fuji Photo Film Co Ltd, Japan SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08122960	A	19960517	JP 1994-263792	19941027 <
JP 3505240	B2	20040308		
PRIORITY APPLN. INFO.:			JP 1994-263792	19941027

AB The claimed photog. material having, on a support, >1 light-sensitive Ag halide emulsion layer(s) contains an imidazole compound substituted by an anilino group (H atom on NH group is unsubstituted) at 2- or 4-site. Preferable imidazole derivative is represented by the formula I (RI-4 = H, nonmetal substituent; X = OH, NRSRG R, PS, R6 = H, alkyl, aryl,

heterocyclic group; A, B = nonmetal substituent). The compound is a leuco dye with high dye developability and the developed dye has a high spectral absorbance.

IT 179421-93-3P

RL: DEV (Device component use); PNU (Preparation, unclassified); PREP (Preparation); USES (Uses)

(silver halide photog. material containing anilinoimidazole to develop dye image with high spectral absorption)

RN 179421-93-3 CAPLUS

CN

Pentanamide, N-[4-[2-(acetylamino)phenyl]-5-[[4-(diethylamino)-2methylphenyl|amino|-1H-imidazo1-2-v1|- (CA INDEX NAME)

L15 ANSWER 16 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:183280 CAPLUS DOCUMENT NUMBER: 122:55805

ORIGINAL REFERENCE NO.: 122:10814h,10815a

TITLE: A Simple and Practical Synthesis of 2-Aminoimidazoles

AUTHOR(S): Little, Thomas L.; Webber, Stephen E.

CORPORATE SOURCE: Agouron Pharmaceuticals Inc., San Diego, CA, 92121,

Journal of Organic Chemistry (1994), 59(24), SOURCE:

7299-305 CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 122:55805

AB A new and simple two-step procedure to synthesize 2-aminoimidazoles (2-AI's) from readily available materials has been developed. The cyclization reaction of α -halo ketones RCOCHR1X [R = Me, Et, CMe3, Ph, 4-BrC6H4, etc., R1 = H, Me, Ph, RR1 = (CH2)3, (CH2)4, X = C1, Br] and N-acetylguanidine in acetonitrile (MeCN) at reflux, or in DMF at ambient temperature, gives 4(5)-substituted and 4,5-disubstituted N-(1H-imidazo1-2-y1)acetamides I, which are then hydrolyzed to their resp. 2-AI's. In general, the purified products were isolated in good yields. We have prepared several examples and have demonstrated the usefulness of this method by its application in the total synthesis of 2-aminohistamine, an interesting histamine analog, and oroidin (II), a marine natural product isolated from various sponges.

160041-64-5P 160041-65-6P 160041-66-7P 160041-67-8P 160041-68-9P 160041-69-0P

160072-51-5P 160072-52-6P 160072-53-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of aminoimidazoles, aminohistamine, and oroidin by cyclization of carbonyl with acetylguanidine)

160041-64-5 CAPLUS RN

CN Acetamide, N-(5-phenyl-1H-imidazol-2-yl)- (CA INDEX NAME)

RN 160041-66-7 CAPLUS

CN Acetamide, N-[5-(4-bromophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 160041-67-8 CAPLUS

CN Acetamide, N-[5-(4-methoxyphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 160041-68-9 CAPLUS

CN Acetamide, N-[5-(3-nitrophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 160041-69-0 CAPLUS

CN Acetamide, N-[5-(3-phenoxyphenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RN 160072-51-5 CAPLUS

CN Acetamide, N-(4-methyl-5-phenyl-1H-imidazol-2-yl)- (CA INDEX NAME)

RN 160072-52-6 CAPLUS

CN Acetamide, N-(4,5-diphenyl-1H-imidazol-2-yl)- (CA INDEX NAME)

RN 160072-53-7 CAPLUS

CN Acetamide, N-[5-(2-naphthalenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

L15 ANSWER 17 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:540469 CAPLUS DOCUMENT NUMBER:

117:140469

ORIGINAL REFERENCE NO.: 117:24183a,24186a

TITLE: Cyan coupler-containing photographic material

INVENTOR(S): Nakayama, Noritaka; Uchida, Taku; Masukawa, Toyoaki Konica Co., Japan PATENT ASSIGNEE(S):

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATEN'	r no.	KIND	DATE	APPLICATION NO.	DATE
JP 03:	284746	A	19911216	JP 1990-86760	19900330 <
PRIORITY A	PPLN. INFO.:			JP 1990-86760	19900330
AB In the	e title photog	g. mater	ial contain	ing ≥1 Ag halide emulsion	on layers,
≥1 of	the Ag halide	e emulsi	on layer co	ntains a cyan coupler (I) [R =
H, su	ostituent; L :	= divale	nt linking	group; R1 = proton donor	r which may
H-bone	d with N of th	ne parer	t ring; R2	= substituent; $m = 1-4$;	X = H, group
relea	sable on coup.	ling wit	h an oxidiz	ed color developing ages	nt]. The cyan
dye p	roduced by th:	is coupl	er has good	spectral absorption cha	aracteristics
with:	sharp cutoff a	at the s	hortwave si	de, unsym. absorption is	s not observed in
the b	lue and green	regions	, and color	reproducibility is supe	erior.
IT 14331	5-84-1P				

RL: PREP (Preparation)

(preparation of, as photog, cvan coupler)

RN 143316-84-1 CAPLUS

Butanamide, N-[2-[2-(acetylamino)-5-chloro-1H-imidazol-4-y1]-4ethoxyphenyl]-2-[2,4-bis(1,1-dimethylpropyl)phenoxy]-3-methyl- (CA INDEX NAME)

L15 ANSWER 18 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1992:13220 CAPLUS DOCUMENT NUMBER: 116:13220

ORIGINAL REFERENCE NO.: 116:2279a,2282a

TITLE: Heat developable color photographic material INVENTOR(S): Miura, Akio; Masukawa, Toyoaki; Komamura, Tawara

PATENT ASSIGNEE(S): Konica Co., Japan Jpn. Kokai Tokkyo Koho, 31 pp.

SOURCE: CODEN: JKXXAF

DOCUMENT TYPE: Pat.ent.

LANGUAGE: Japanese FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03089343 PRIORITY APPLN. INFO.:	A	19910415	JP 1989-227154 JP 1989-227154	19890901 < 19890901

- AR The title material on a support comprises photosensitive silver halide, a reducing agent, a binder, and cyan dye-forming coupler I (A, B = organic group connected to the imidazole ring by the C, N, O, or S atom; X = H, group which is released upon coupling reaction with the oxidized form of the reducing agent). I (A = Q1, B = Q2; X = Q3) is an example of the general structure I defined above. The use of I provides stable cyan dyes and gives excellent cyan dye images.
- 137590-60-4 RL: USES (Uses)
 - (cyan dye-forming coupler, in photog. material)
- RN 137590-60-4 CAPLUS
- CN Propanoic acid, 3-[[4-[2-[[2-[2,4-bis(1,1dimethylpropyl)phenyl]acetyl]amino]phenyl]-2-[(1-oxopentyl)amino]-1Himidazol-5-vl|thio|- (CA INDEX NAME)

$$\begin{array}{c} O \\ H \\ N \\ \end{array}$$
 R
$$\begin{array}{c} H \\ N \\ \end{array}$$
 S
$$\begin{array}{c} CH_2 - CH_2 - CO_2H \\ \end{array}$$

L15 ANSWER 19 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1990:408016 CAPLUS

DOCUMENT NUMBER: 113:8016

ORIGINAL REFERENCE NO.: 113:1505a,1508a

TITLE: Imidazole dyes for thermal-transfer printing inks INVENTOR(S): Uchida, Taku; Masukawa, Toyoaki; Nakayama, Noritaka

PATENT ASSIGNEE(S): Konica Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.

DOCUMENT TYPE: CODEN: JKXXAF
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02028264	A	19900130	JP 1988-177357	19880715 <
PRIORITY APPLN. INFO.:			JP 1988-177357	19880715
OTHER SOURCE(S).	MARPAT	113:8016		

The title dyes, with lower undesired absorption than indoaniline dyes and better heat and light resistance than cyanine dyes, have the general formula I [R1, R2 = H, (un) substituted alky1, R1, R2 = 5 - or 6-membered ring member; R3-6 = H, halogen, (un) substituted alky1, alkoxy; R7 = H, (un) substituted alky1, ary1, R11C0, R1103C2, R12NHSC0, R13R14NC0, R11S02, R1108C2, R12NHSC2, R13R14NSC2; R11 = H, (un) substituted alky1; R12 = (un) substituted alky1, heterocyclic, R13, R14 = (un) substituted alky1; X = CO, SO2, NHCC; R8 = (un) substituted alky1, Y, R9, R10 = monovalent group; n = 0-4; n = 0-5]. Benzaldehyde guany1 hydrazone and 2-[2-(2,4-di-tert-amy1phenoxy) isopentanamido] phenacylbromide in CHC13 were refluxed for 10 min and stirred at room temperature for 1 h to give 2-benzylidenehydrazino-4-[2-[2-(2,4-di-tert-

amylphenoxy)isopentanaido]phenyl]imidazole, which was stirred with Zn/HCl in acetone to give 2-amino-4-[2-[2-(2,4-di-tert-

amylphenoxy)isopentamido]phenyl]imidazole. This product was treated with BzCl in the presence of NaOAc in EtOAc to give

2-amino-3-benzoy1-4-[2-[2-(2,4-di-tert-

amylphenoxy)isopentanamido]phenyl]imidazole, which was then heated with p-MeC6H4S03H in PhNO2 at 150° for 1 h to give

2-benzoylamino-4-[2-[2-(2,4-di-tert-

amylphenoxy)isopentanamido]phenyl]imidazole, which was then dissolved in EtOAc, stirred with aqueous K2CO3, treated with aqueous

4-amino-3-methyl-N-methyl-N-(β-methanesulfonamidomethyl)aniline

sulfate, then with 10% aqueous K2S2O8 to give I [R1 = Et; R2 = CH2Ch2NHSO2Me; R2 = Me; R4 = R5 = R6 = R9 = H; R7 =

2-(2,4-di-tert-amylphenoxyispropanoyl)].

127698-35-5P RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT

(Reactant or reagent)

(manufacture and reaction of, with aniline derivs.)

RN 127698-35-5 CAPLUS

CN Butanamide, N-[2-[2-(acetylamino)-1H-imidazol-5-yl]phenyl]-2-[2,4-bis(1,1dimethylpropyl)phenoxy]-3-methyl- (CA INDEX NAME)

L15 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1987:32967 CAPLUS

DOCUMENT NUMBER: 106:32967

ORIGINAL REFERENCE NO.: 106:5527a,5530a

TITLE:

Heterocyclic rearrangements. Rearrangement of N-(1,2,4-oxadiazol-3-vl)-β-enamino ketones to

pyrimidine N-oxides

AUTHOR(S):

Vivona, Nicolo; Buscemi, Silvestre; Frenna, Vincenzo; Ruccia, Michele

CORPORATE SOURCE: Inst. Org. Chem., Univ. Palermo, Palermo, 90123, Italy SOURCE: Journal of the Chemical Society, Perkin Transactions

1: Organic and Bio-Organic Chemistry (1972-1999) (

1986), (1), 17-19 CODEN: JCPRB4: ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

(preparation of)

CASREACT 106:32967

OTHER SOURCE(S): AB

The behavior of oxadiazolylenamino ketones I (R, R1 = Me, Ph; R2 = Me, Ph, OEt) towards rearrangement has been investigated. In the presence of anionic reagents in ethanol solution, they rearrange to pyrimidine N-oxides

II (R3 = Me, Ph). The synthesis and hydrolytic ring opening of an oxadiazolopyrimidinium system III is also reported.

55729-99-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

RN 55729-99-2 CAPLUS

CN 1H-Imidazole-4-carboxylic acid, 2-(acetylamino)-5-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

L15 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1985:185082 CAPLUS DOCUMENT NUMBER: 102:185082 CAPLUS ORIGINAL REFERENCE NO.: 102:29037a,29040a

TITLE: Amidine derivatives of 2-substituted 4-phenylimidazole

INVENTOR(S): Bietti, Giuseppe; Cereda, Enzo; Donetti, Arturo;

Giachetti, Antonio; Pagani, Ferdinando PATENT ASSIGNEE(S): Istituto De Angeli S.p.A., Italy

SOURCE: Eur. Pat. Appl., 43 pp.

CODEN: EPXXDW
DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	TENT NO.			KIND	DATE	APPLICATION NO.			DATE			
EP	131973 131973			A1	19850123 19890802	EP	1984-200659		19840508	<		
	R: AT,	BE,	CH,	DE, F	R, IT, LI,	LU, N	L, SE					
AT	45149			T	19890815	AT	1984-200659		19840508	<		
US	4649150			A	19870310	US	1984-610958		19840516	<		
FI	8402432			A	19850119	FI	1984-2432		19840615	<		
JP	60038367			A	19850227	JP	1984-142099		19840709	<		
DD	232696			A5	19860205	DD	1984-265319		19840716	<		
PL	143303			B1	19880229	PL	1984-248779		19840716	<		
IL	72417			A	19880331	IL	1984-72417		19840716	<		
PL	143732			B1	19880331	PL	1984-254625		19840716	<		
DK	8403500			A	19850119	DK	1984-3500		19840717	<		
NO	8402921			A	19850121	NO	1984-2921		19840717	<		
NO	162857			В	19891120							
NO	162857			C	19900228							
	34959			A2	19850528		1984-2781		19840717	<		
HU	193292			В	19870928							
GB	2149395			A	19850612	GB	1984-18149		19840717	<		
	2149395			В	19861126							
	8405490			A	19860326		1984-5490		19840717			
	1322979			A3	19870707		1984-3770847					
	1257274			A1	19890711		1984-459030		19840717			
	8430800			A	19850124		1984-30800		19840718	<		
	565292			B2	19870910							
	244141			B2	19860717		1984-5542		19840718			
	1313345			A3	19870523		1985-3844125		19850129			
	244150			B2	19860717		1985-2801		19850416	<		
PRIORITY	Y APPLN.	INFO.	. :				1983-22110		19830718			
							1984-200659		19840508			
							1984-5542	A3	19840718			

OTHER SOURCE(S): MARPAT 102:185082

AB Forty-four (amidinophenyl)imidazoles I [R = alkyl, OH, alkoxy, SH, alkylthio, halo, alkylsulfinyl, alkylsulfonyl, SO2NH2, (di)(alkyl)amino, acylamino, Ph; Rl, R2 = H, alkyl; R3 = alkyl optionally containing 1 hetero atom such as O, S, or N, alkenyl, alkynyl, cyano, cycloalkyl, cycloaliph.

alkyl, (un) substituted aryl, aralkyl, heterocyclylalkyl, heterocyclyl; R4 = H, alkyl, alkoxy, halo, cyano, CONH2] were prepared Thus, 4-O2NC6H4COCH2Br in water was treated with AcNH2 at 140° for 8 h to give phenylimidazole II (R5 = NO2), which was catalytically reduced to II (R5 = NH2). The latter compound was condensed with EtOCH:NCN to give II (R5 = N:CHNHCN), which was treated with EtNH2 to give II (R5 = N:CHNHEt)(III). III inhibited histamine-induced tachycardia in isolated guinea pig atria with an EC50 of 1.5 + 10-7M.

96139-96-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with isopropylamine)

RN 96139-96-7 CAPLUS

CN Acetamide, N-[5-[4-[[(cyanoamino)methylene]amino]phenyl]-1H-imidazol-2-yl]-(CA INDEX NAME)

96139-70-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reduction of)

RN 96139-70-7 CAPLUS

CN Acetamide, N-[5-(4-nitrophenyl)-1H-imidazol-2-yl]- (CA INDEX NAME)

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of) RN 96154-06-2 CAPLUS

CN Acetamide, N-[4-[4-[[[(1-methylethyl)amino]methylene]amino]phenyl]-1Himidazol-2-yl]-, (2Z)-2-butenedioate (1:2) (9CI) (CA INDEX NAME)

CM 1

CRN 96154-05-1 CMF C15 H19 N5 O

CM

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

IT 96139-64-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, hydride reduction, and reaction of, with cyanoformimidate)

RN 96139-64-9 CAPLUS

CN Acetamide, N-[5-(4-aminophenyl)-1H-imidazo1-2-yl]- (CA INDEX NAME)

L15 ANSWER 22 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1975:112006 CAPLUS

DOCUMENT NUMBER: 82:112006

ORIGINAL REFERENCE NO.: 82:17899a,17902a

TITLE: Mononuclear heterocyclic rearrangements. VI.
Conversion of 1,2,4-oxadiazoles into imidazoles

AUTHOR(S): Ruccia, M.; Vivona, N.; Cusmano, G.
CORPORATE SOURCE: Fac. Sci., Univ. Palermo, Palermo, Italy

SOURCE: Tetrahedron (1974), 30(21), 3859-64 CODEN: TETRAB; ISSN: 0040-4020

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 82:112006

AB Condensation of aminooxadiazoles with β-oxo ketones or esters gave β-enamino ketones, which with NaOEt in DMF rearranged to imidazole derivs. E.g., I with (MeCO)2CH2 gave II, which with NaOEt in DMF gave III. Condensation of I with PhCOCH2CO2Et gave IV and V. V was in solution equilibrium with its tautomer VI.

IT 55729-99-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 55729-99-2 CAPLUS

CN 1H-Imidazole-4-carboxylic acid, 2-(acetylamino)-5-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

L15 ANSWER 23 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1962:46003 CAPLUS DOCUMENT NUMBER: 56:46003

ORIGINAL REFERENCE NO.: 56:8702f-i.8703a-e

TITLE: 2-Phenylhydrazinoimidazoles and their benzidine-like

rearrangement

AUTHOR(S): Pyl, Theodor; Lahmer, Helmut; Beyer, Hans

CORPORATE SOURCE: Univ. Greifswald, Germany

SOURCE: Chemische Berichte (1961), 94, 3217-23

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 56:46003

PhNHC(:NH)NH2 (I) reacts with BzCH2Br (II) and its aryl analogs to yield the corresponding 2-phenylhydrazinoimidazoles (III) which undergo with concentrated HCl a benzidine-like rearrangement. The structure was proved by the rearrangement of 2-phenylhydrazino-4(5)-phenylimidazole (IV) to 2-amino-4-phenyl-5-(p-aminophenyl)imidazole (V) and subsequent deamination to the known 2-amino-4,5-diphenylimidazole (VI). The lack of reducing properties in the III indicates the presence of the tautomeric 2-imidazolone phenylhydrazone form. I.HCl (3.73 g.) in 25 cc. MeOH treated with cooling with 0.46 g. Na in 20 cc. MeOH, filtered, and treated with 2 g. II in Me2CO gave 1.5 g. IV, needles, m. 225-6° (decomposition) (BuOH), turned yellow to pink in air; IV.HCl, rodlets, m. 201° (decomposition) (BuOH). IV refluxed 1 hr. with excess Ac2O in C5H5N gave the di-Ac derivative (VII) of IV, leaflets, m. 232° (decomposition) (1:1 BuOH-EtOH); di-Bz derivative, yellowish powder, decomposing above 230° with darkening. I.HCl (3.73 g.) and 2.78 g. p-BrC6H4COCH2Br gave 1.5 g. 4(5)-p-BrC6H4 analog (VIII) of IV, needles, m. 227° (decomposition) (BuOH); VIII.HCl, rodlets, m. 215° (decomposition); di-Ac derivative of VIII, yellowish microcryst. powder, m. 155-6° (aqueous EtOH). I.HCl (3.73 g.) with 1.86 g. p-MeC6H4COCH2C1 gave 1.5 g. 4(5)-p-MeC6H4 analog (IX) of IV, needles, m. 223-4°, (BuOH); IX.HCl, rodlets, m. 198° (decomposition); di-Ac derivative of IX, rodlets, m. 272-3° (aqueous EtOH). I.HCl (3.73 g.) with 2.3 g. p-MeOC6H4COCH2Br yielded 1.6 g. 4(5)-p-MeOC6H4 analog of IV, needles, m. 215-16° (decomposition); IV.HCl, rodlets, m. 213- 14° (decomposition) (BuOH); di-Ac derivative, yellowish crystal powder, m. 172-3°. IV (0.5 g.) in 3 cc. o-HOC6H4CHO refluxed briefly, cooled, diluted with 2 vols. EtOH, and filtered gave nearly 100% 4-phenyl-5-salicylidene-2-imidazolone phenylhydrazone (X), yellow needles, m. 230° (decomposition) (EtOH). Similarly were prepared the following 4-aryl analogs of X (aryl group and m.p. given): p-BrC6H4 213° (decomposition) (EtOH), p-MeC6H4 234° (decomposition) (EtOH); p-MeOC6H4 211° (decomposition) (EtOH); all yellow needles. VII (4 g.) and 40 cc. concentrated HCl refluxed 5 hrs., concentrated

beginning crystallization, cooled, and filtered gave 2 g. V.2HCl, needles, m. 310° (decomposition). IV (30 g.) and 250 cc. concentrated HCl refluxed, and the precipitate dissolved in a little H2O and repptd. with concentrated HCl ave 8 g.

V.2HCl, needles, m. 310° (decomposition). V.2HCl in H2O treated with NH4OH gave V, yellowish rodlets, m. 265° (decomposition). V and excess Ac2O refluxed 1 hr. gave the di-Ac derivative, needles, m. 261° (EtOH). VIII (25 g.) in 250 cc. concentrated HCl refluxed 5 hrs., cooled, decanted from some resin, kept some time, filtered, and concentrated, and the precipitate dissolved

in a little cold H2O and repptd. with concentrated HCl gave 3 g. 4-(p-BrC6H4) analog (X.2HCl) of V.2HCl, needles, m. 220° (decomposition). X.2HCl in H2O treated with dilute NH4OH gave X, powder, decomposing above 310° (aqueous EtOH). IX (26 g.) yielded similarly 8 g. 4-(p-MeC6H4) analog of

V.2HCl, needles, m. 305°; free base, colorless prisms, decompose

303°; di-Ac derivative, yellowish crystal powder, m. 296°

(EtOH). V (2 g.) in 5 cc. concentrated HCl and 50 cc. H2O treated at 0°

with 0.6 g. NaNO2 in 5 cc. H2O and added to 1 g. 2-C10H7OH in 100 cc. 20% aqueous NaOH, and the violet flocculent precipitate washed with H2O, dissolved in 100

cc. hot EtOH, filtered, and diluted with H2O and a few drops HCl gave 0.8 g. 5-[p-(2-C10H7N:N)C6H4] analog of V, brown-violet powder, decomposing at higher temperature without melting, red-violet in organic solvents.

Diazotized V

added to aqueous H3PO2, and the crystalline precipitate crystallized from

dilute HCl, dissolved

in MeOH, treated with dilute aqueous NaOH, and diluted with H2O yielded VI, prisms, m. 243° (decomposition).

98783-56-3P, Acetanilide, 4'-[2-acetamido-5(or

4)-phenylimidazol-4-(or 5)-y1]- 99080-81-6P, Acetanilide, 4'-[2-acetamido-5(or 4)-p-tolylimidazol-4-(or 5)-yl]-

RL: PREP (Preparation) (preparation of)

98783-56-3 CAPLUS RN

CN Acetanilide, 4'-[2-acetamido-5(or 4)-phenylimidazol-4(or 5)-v1]- (7CI) (CA INDEX NAME)

99080-81-6 CAPLUS RN

Acetanilide, 4'-[2-acetamido-5(or 4)-p-tolylimidazol-4(or 5)-yl]- (7CI) (CA INDEX NAME)

L15 ANSWER 24 OF 24 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1919:6989 CAPLUS 13:6989

DOCUMENT NUMBER:

ORIGINAL REFERENCE NO.: 13:1301f-i,1302a-i,1303a-i,1304a-b TITLE: Nitro-, arylazo-, and aminoglyoxalines

Fargher, Robert George; Pyman, Frank Lee AUTHOR(S): CORPORATE SOURCE: Welcome Chem. Res. Lab., London

SOURCE: Journal of the Chemical Society, Transactions (

1919), 115, 217-60

CODEN: JCHTA3; ISSN: 0368-1645

DOCUMENT TYPE: Journal

cf. C. A. 10, 1631. All m. ps. are corr. The object of this investigation was to prepare purine derivs. by building up a pyrimidine ring upon a glyoxaline nucleus, a method complementary to the usual one. It was proposed to prepare 4-aminoglyoxaline-5-carboxylic acid, CH:N.C(NH2):C(CO2H).NH, condense it with HCNO and obtain xanthine. The synthesis was not accomplished because of inability to obtain the starting material. I. The preparation of glyoxalines and their carboxylic acids: Glvoxaline-4,5-dicarboxvlic acid (a), prepared in 60% vield by mixing cold aqueous solns, of nitrotartaric acid and CH2O, m. 288° (decomposition). Mono-sodium salt, forms feathery needles containing 1 H2O. Glyoxaline (b) is prepared by distilling (a) in small quantities at a time; picrate, yellow needles containing 1 H2O, m. 212°; hydrogen tartrate, anhydrous prisms, m. 202°; hydrogen oxalate, anhydrous prismatic needles, m. 232°. On heating (a) to above 180° with H2o or HCL the main product is (b) with a little glyoxaline-4-carboxylic acid. When (a) is heated to 180-200° with concentrated NH4OH the main product is (b). On boiling (a) with PhNH2 the main product is glyoxaline-4-carboxanilide, anhydrous needles, m. 227-8°, hydrolyzed by 10% HCl at 130°, producing glyoxaline-4-carboxylic acid. 2-Methylglyoxaline-4,5-dicarboxylic acid (c) is prepared from AcH and nitrotartaric acid in 67% vield. On boiling (c) with PhNH2 there is obtained 11 g. 2-methyl-glyoxaline-4-carboxanilide (d), m. 208°, and 3.8 g. 2-methylglyoxaline; picrate, anhydrous needles from H2O, m. 213°; hydrogen oxalate, rhombic prisms from H2O containing 2 H2O; after drying at 100° it m. 160°. Hydrolysis of (d) gives 2-methylglyoxaline-4-carboxylic acid as a monohydrate, prismatic needles, m. 262° (decomposition); nitrate, rhombic prisms from H2O, m. 190°; picrate, minute cubes containing 2H2O, m. 200°. 2-Ethylglyoxaline-4,5-dicarboxylic acid, prepared from EtCHO and nitrotartaric acid in 64% yield, m. 259° (decomposition). 2-Phenylglyoxaline-4,5-dicarboxylic acid, from BzH and nitrotartaric acid in 48% yield, m. 2710 (decomposition). When distilled in small quantities it gives an 80% yield of 2-phenylglyoxaline, needles from H2O, m. 148-9°; nitrate, leaflets from alc. containing 0.75 H2O, m. (dry) 135°; hydrogen oxalate, needles, m. 219° (decomposition); picrate, fine needles, m. 238°. Upon mixing 8.6 g. Ac2 in 50 cc. H2O, 50 cc. of 40% aqueous CH2O, and 80 cc. concentrated NH4OH at 0° there is obtained after standing in a cool place overnight, evaporating to a small bulk, saturating with K2CO3, extracting with Et2O, and evaporating the extract, 5.9 g. of an oil which is boiled with dilute HCl to destroy C6H12N4 and separated by fractionating the picrates from H2O into 5.7 g. 4.5-dimethylglyoxaline picrate (e), and 3.5 g. 2,4,5-trimethylqlyoxaline picrate, m. 163°. 4,5-Dimethylglyoxaline hydrochloride forms rhombic prisms from H2O, m. 305° (decomposition). (e) is also prepared from MeCOC(:NOH)Me (9 g.) by reducing with SnCl2 at is 15° and evaporating the final liquor under reduced pressure; the resulting 10 g. MeCOCH (NH2) Me heated on the H2O bath 4 hrs. with 10 g. KCNS and 40 cc. H2O gives 5.2 g. 2-thiol-4,5-dimethylglyoxaline and the latter gives an 85% yield of (e) when oxidized with the calculated quantity of FeCl3. II. Nitroglyoxalines: 4-Nitroglyoxaline (f) is obtained in 63% yield when 8 g. of (b) in 16 cc. cold ${\rm HNO3}$ (1.4), is cautiously treated with 16 cc. ${\rm H2SO4}$, and after the vigorous reaction is over boiled 2 hrs. and poured into ice- ${\rm H2O}$.

4-Nitro-2-methylglyoxaline, (g), prepared similarly, anhydrous needles from

4,5-dimethylglyoxaline (5 g.) with HNO3 and H2SO4 1.7 g. was recovered

H2O, sinter 251°, m. 254°. On nitrating 4-methylglyoxaline by the method of Windaus (C. A. 3, 1268) the main product is 4-methylglyoxaline nitrate instead of 5-nitro-4-methylglyoxaline (h) as stated by him. (h), obtained in 90% yield by the method described for

preparing (g), m. 248°. On attempting to nitrate

4-methylglyoxaline-5-carboxylic acid. When (f), (g), or (h) are reduced with Sn and HCl two of the three atoms of N present are eliminated as NH3. Three mols. (f) on reduction with alkaline Na2S2O4 loses 2 atoms N as NH3. The remaining liquor gradually acquired a blue color as noted by Behrend and Schmitz (Ann. 277, 338) and on acidification precipitated less than 0.1 q. a blue compound m. above 300°. (h) on reduction behaved analogously but gave a rose color and no precipitate (g) gave 1 mol. of NH3 from 3 mols. of the nitro-compound III. Arvlazoglyoxalines: In the opinion of the authors it appears that glyoxalines, in order to be capable of coupling, must contain a free « NH group and also a H atom or some other displaceable group, such as CO2H, in one of the 2-, 4-, or 5-positions. All previously prepared arylazoglyoxalines are C-azo compds. In general, the monoarylazoglyoxalines are soluble in alc., EtOAc and Me2CO, sparingly soluble in Et20, CHC13 and C6H6, insol, in cold H2O and dilute alkali, form soluble salts with dilute HCl; are decomposed by boiling 1 hr. with 10% HCl, give bright colors with concentrated H2SO4. 17 g. (b) and 40 g. Na2CO3 in 125 cc. H2O treated at 5° with a diazotized solution of 23.25 g. PhNH2 give an orange powder which, on extracting with cold 2.5% HCl, left 4.4 g. residue of 2,4,5-trisbenzeneazoglyoxaline, decomps. about 200°, effervesces 208°. The HCl extract made alkaline gave 34 g. 2-benzeneazoglyoxaflne (i), m. 190°, 20 g. of (i) reduced with SnC12 gives 3.2 g. 2-aminoglyoxaline, chlorostannate, a trace of NH2C(:NH)NH2, and 18.55 g. 2-amino-4-p-aminophenylglyoxaline dihydrochloride (j), formed by rearrangement of the benzidine type, m. above 300°; free base, formed by boiling with Na2CO3, glistening leaflets containing 1 H2O, m. 148°; dipicrate, yellow needles, darken 245°, M. 250° (decomposition). 2-Acetylamino-4-p-acetylaminophenylglyoxaline, by boiling the base with Ac20 1 hr., crystalline powder, m. above 300°. 10 g. in dilute H2S04 with 4% KMnO4 gave 1 g. p-AcNHC6H4CO2H, m. 260°. Reduction of 17.2 g. (i) with Zn dust and AcOH gives a small amount of (i), 7 g. PhNH2, and 5.9 g. of pure glycocyamidine hydrochloride (k), sintered 205°, m. 211-3°; free base, prismatic needles. begins darkening 220° and does not m. 300°; chloroplatinate, C3H5ON3.H2PtC16.2H2O, darkens 220°, entirely black at 260°, does not m. 300°; chloraurate, C3H5ON3.AuCl3, m. 157-8°; picrate, yellow leaflets, m. 215-16°. By treating 13.6 g. (b) in Na2CO3 at 5° with a diazotized solution of 34.4 g. p-BrC6H4NH2 there resulted 48.7 g. crude 2-p-bromobenzeneazoglyoxaline (1); crystallization from alc. gave 42.6 g. of the pure compound m. 253° (decomposition) and a small amount of 4-p-bromobenzeneazoglyoxaline, m. 191° (decomposition). (1) (78 g.) on reduction with SnC12 gave 40.7 g. p-BrC6H4NH2, 2.7 g. of 2-amino-4-p-aminophenylglyoxaline, isolated as the picrate, 1.6 g. NH2C(:NH)NH2.(CO2H)2, m. 173-4°, 0.9 g. of a base forming needles, m. 178°, probably having the structure 5,2-Br(H2N)C6H3NHC:N.CH:CH.NH, and 20.7 g. 2-aminoglyoxaline hydrochloride (m), plates from alc., m. 152°; free base, obtained as a colorless sirup by adding 1 equivalent of Na2CO3, evaporating to dryness, extracting and evaporating the alc.; chlorostannate, prismatic needles, m. 286°; nitrate, transparent tablets, sinter 125°, m. 135-6°; hydrogen oxalate, tablets, m. 211°; picrate, silky needles, m. $2\ddot{3}6^{\circ}.$ 2-Acetylaminoglyoxaline, prepared by boiling (m) with Ac2O and AcONa, prisms, sinter $270^{\circ},$ m. $287^{\circ}.$ 2-Benzoylaminoglyoxaline, prepared by Schotten-Baumann reaction, leaflets, m. 227°. 4-Methylglyoxaline (32.8 g.) in NaHCO3 treated with PhN:NCl gave 17.3 g. 2,5-bisbenzeneazo-4-methylgtyoxaldne, garnet-red needles from alc., m. 206° (decomposition); 17 g. of 5-benseneazo-4-methylglyoxaline (n), copper-colored needles, m.

unchanged and the only product was 0.3 g. of the nitrate of

of

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240° (decomposition); 7.4 q. of 2-benzeneazo-4-methylglyoxatine (o),
 orange prisms, m. 185°. Reduced with SnC12 (o) gives
 2-amino-5-p-amixophenyl-4-methylglyoxaline dihydrochloride (p),
 diamond-shaped plates, m. above 300°. (p) boiled with Na2CO3 gives
 the monohydrochloride, flat needles, sinter 80°, m. 260°;
 dipicrate, yellow needles, m. 255°.
 2-Acetylamino-5-p-acetylaminophenyl-4-methylglyoxaline hydrochloride,
 prepared by the action of Ac20 and AcONa on (p), needles containing 4 H2O,
 after drying at 100° m. 303° (decomposition). On adding NH4OH to
 the solution of the hydrochloride the free base is precipitated, needles, m.
 280°. 2-Amino-5-p-benzylideneaminophenyl-4-methylglyoxali
 neacetate, prepared by adding BzH to (p) in AcONa solution, m. 208°. (o)
 on reduction with Zn and AcOH gave 1.4 g. brown sirup from which was separated
 a small quantity of the dipicrate of (p) and about 0.7 g. alacreatinine
 hydrochloride, prisms, m. 202-3°; free base, m. 222-3°;
 picrale, yellow needles, sinter 200°, m. 212°. On reduction
 of 14 g. of (n) with SnC12 there is obtained besides PhNH2 and a brown
 qum, 2.2 q. of the hydrochloride, C9H10ON2.HCl, rectangular tablets, m.
 308°, from which a base, C3H10ON2, is obtained by adding NH4OH and
 crystallizing from H2O, prisms, m. 185°. Reduction of 10. q. (n) with Zn
 and AcOH produced 5.5 g. of a varnish-like substance and 1.6 g. of the
 base C10HON3, small, rhomboidal plates, m. 265°; hydrochloride,
 oblong plates, m. 206-8°, decomposed by heating 2.5 hrs. at
 170° into NH4Cl and a hydrochloride, m. about 280°.
 2-Methylglyoxaline in Na2CO3 treated with PhN:NC1 gives a product which
 easily resinifies and from which a small amount of
 4-benzeneazo-2-methylglyoxaline was obtained pure, m. 158°.
 4-p-Bromobenzeneazo-2-methylglyoxaline, prepared in good yield from
 2-methylglyoxaline in Na2CO3 and p-BrC6H4N:NCl, red prism sfrom absolute alc.,
 m. 2000 (decomposition); reduction with either SnCl2 or Zn and AcOH give
 no definite products. 2-Phenylglyoxaline (7.2 g.) heated with
 p-BrC6H4N:NCl gives 13 g. 2-phenyl-4-p-bromobenzeneazoglyoxaline (g),
 orange needles, m. 201°. Reduction of (g) with SnCl2 gives a
 crystalline hydrochloride, C15H13N4Br.2HCl, m. 255°; triacetyl
 derivative, formed by heating with Ac2O and AcONa, m. above 300°.
 This base is probably the result of a change of the semidine or benzidine
 type. 2-p-Sulfobenzeneazoglyoxaline-4,5-dicarboxylic acid, prepared by
 treating glyoxaline-4,5-dicarboxylic acid with SO3HC6H4N:NCl, red prisms
 containing 2 H2O which are lost at 130° in vacao; disodium salt
 (r), yellow, silky needles containing 3 H2O. Reduction of 6.2 g. (r) with
 Na2S2O4 gives 1.6 g. of 2-aminoglyoxaline-4,5-dicarboxylic acid, pale buff
 needles, effervesce 245° and then melt. On boiling 6 hrs. with
 PhNH2 the product was identified as (m).
861294-61-3P, Imidazole, 2-acetamido-4-(p-acetamidophenyl)-
 861325-21-5P, Imidazole, 2-acetamido-5-(p-acetamidophenyl)-4-
 methyl-, hydrochloride 861325-23-7P, Acetanilide,
```

(preparation of) RN 861294-61-3 CAPLUS

RL: PREP (Preparation)

p-(2-acetamido-4-methyl-5-imidazolyl)-

TT

CN Acetamide, N-[4-[2-(acetylamino)-1H-imidazol-5-yl]phenyl]- (CA INDEX NAME)

RN 861325-21-5 CAPLUS

CN Acetamide, N-[4-[2-(acetylamino)-4-methyl-1H-imidazol-5-yl]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

HC1

RN 861325-23-7 CAPLUS

CN Acetamide, N-[4-[2-(acetylamino)-4-methyl-1H-imidazol-5-yl]phenyl]- (CA INDEX NAME)

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DICTIONARY FILE UPDATES: 24 OCT 2008 HIGHEST RN 1065816-63-8

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L18 STRUCTURE UPLOADED

=> que L18

L19 QUE L18

=> d 119

L19 HAS NO ANSWERS L18 STR

Structure attributes must be viewed using STN Express query preparation. L19 OUE ABB=ON PLU=ON L18

=> s 119 sss full

FULL SEARCH INITIATED 11:55:21 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED -599 TO ITERATE

100.0% PROCESSED 599 ITERATIONS

SEARCH TIME: 00.00.01

14 ANSWERS

L20 14 SEA SSS FUL L18

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```
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SQD - Protein sequence data, includes RN
      - Same as SQD, but 3-letter amino acid codes are used
SOD3
SQN
      - Protein sequence name information, includes RN
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PPROP - Table of predicted properties
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are: (RN = CAS Registry Number)
      - RN
REG
SAM
      - Index Name, MF, and structure - no RN
FIDE
      - All substance data, except sequence data
      - FIDE, but only 50 names
```

SQIDE3 - Same as SQIDE, but 3-letter amino acid codes are used

SQIDE - IDE, plus sequence data

SQD - Protein sequence data, includes RN

```
SQD3
      - Same as SQD, but 3-letter amino acid codes are used
SON
      - Protein sequence name information, includes RN
EPROP - Table of experimental properties
PPROP - Table of predicted properties
PROP - EPROP, ETAG, PPROP and SPEC
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     FILE 'REGISTRY' ENTERED AT 11:30:38 ON 27 OCT 2008
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L2
                QUE L1
             22 S L2 SSS FULL
L3
     FILE 'CAPLUS' ENTERED AT 11:31:05 ON 27 OCT 2008
             22 S L3
1.5
             16 S L4 AND PY<=2004
    FILE 'REGISTRY' ENTERED AT 11:40:27 ON 27 OCT 2008
L6
               STRUCTURE UPLOADED
               OUE L6
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             1 S L7 SSS FULL
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=> s 120 L21

12 L20

=> s 121 and py<=2004 25113423 PY<=2004

3 L21 AND PY<=2004

=> d 122 1-3 ibib ab

L22 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:80450 CAPLUS

DOCUMENT NUMBER: 140:145835

TITLE: Preparation of dibenzofused

bicyclo[2.2.2]octane-derived amides as modulators of

the glucocorticoid receptor

INVENTOR(S): Vaccaro, Wayne; Yang, Bingwei Vera; Kim, Soong-hoon; Huynh, Tram; Tortolani, David R.; Leavitt, Kenneth J.; Li, Wenying; Doweyko, Arthur M.; Chen, Xiao-tao;

Doweyko, Lidia

Bristol-Myers Squibb Company, USA; et al. PATENT ASSIGNEE(S):

PCT Int. Appl., 265 pp. SOURCE: CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE:

English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
WO 2004009017 WO 2004009017		WO 2003-US22300	20030717 <
CO, CR, CU,	CZ, DE, DK, DM,	BA, BB, BG, BR, BY, DZ, EC, EE, ES, FI, JP, KE, KG, KP, KR,	GB, GD, GE, GH,
LS, LT, LU,	LV, MA, MD, MG,	MK, MN, MW, MX, MZ, SD, SE, SG, SK, SL,	NI, NO, NZ, OM,
TR, TT, TZ,	UA, UG, US, UZ,	VC, VN, YU, ZA, ZM, SL, SZ, TZ, UG, ZM,	ZW
KG, KZ, MD,	RU, TJ, TM, AT,	BE, BG, CH, CY, CZ, LU, MC, NL, PT, RO,	DE, DK, EE, ES,
BF, BJ, CF,	CG, CI, CM, GA,	GN, GQ, GW, ML, MR, AU 2003-251970	NE, SN, TD, TG
	A1 20040708	US 2003-621909	
EP 1534273	A2 20050601	EP 2003-765638 GB, GR, IT, LI, LU,	
IE, SI, LT,	LV, FI, RO, MK,	CY, AL, TR, BG, CZ, JP 2004-523482	EE, HU, SK
NO 2005000074	A 20050309	NO 2005-74 US 2005-85347	20050106
PRIORITY APPLN. INFO.:	20000001	US 2002-396877P US 2003-621909	P 20020718 A1 20030717
OTHER SOURCE(S):	MARPAT 140:1458	WO 2003-US22300 35	W 20030717

Title compds. I [R-R4 = H, alk(en/yn)yl, alkoxy, aryl, etc.; Z =

carboxamido, alkylamino, etc.] are prepared For instance, 2-amino-4,5-dimethylthiazole is coupled to the acid derived from the cycloaddn. of methacrylic acid and anthracene (CH3CN, EDCI, Et3N, HOAt, 18 h) to give II. I are glucocorticoid receptor modulators which are useful in treating diseases requiring glucocorticoid receptor agonist or antagonist therapy such as obesity, diabetes, inflammatory and immune disorders.

L22 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:80449 CAPLUS

DOCUMENT NUMBER: 140:157927

TITLE: Homology modeling of nuclear hormone receptor Site II

and design of Site II ligands
INVENTOR(S): Doweyko, Arthur; Nadler, Steven G.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 276 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

FAMILY ACC. NUM. COU PATENT INFORMATION:

	PATENT NO.						KIND DATE					ICAT			DATE				
	WO								1					20030717 <					
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			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,	
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	EP	15755	502			A2		2005	0921	- 1	EP 2	003-	7656	37		2	0030	717	
	EP	15755	502			A3		2005	1123										
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	US	20060																717	
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										1	WO 2	003-1	JS22:	299	1	7 2	0030	717	

B. A binding site in nuclear hormone receptors is described and its structural coordinates are provided. The invention provides machine-readable data storage media comprising structure coordinates of Site II and computer systems comprising the machine-readable data storage media. The invention provides methods used in the design and identification of ligands of Site II and of modulators of nuclear hormone receptors. The invention provides ligands of Site II, modulators of NHRs, pharmaceutical compns. comprising modulators of NHRs, methods of modulating NHRs, and methods of treating diseases by administering modulators of an NHR. Also provided are methods of designing mutants, mutant NHRs, Site II binding assays, and models of Site II.

L22 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1981:84008 CAPLUS DOCUMENT NUMBER: 94:84008

ORIGINAL REFERENCE NO.: 94:13701a,13704a
TITLE: Synthesis and halogenation of some new

2-amino-4-substituted imidazoles and their possible

use as pesticides
AUTHOR(S): Nath, J. P.; Mahapatra, G. N.

CORPORATE SOURCE: Dep. Chem., Ravenshaw Coll., Cuttack, 753 003, India

SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1980

), 19B(6), 526-8

CODEN: IJSBDB; ISSN: 0376-4699 Journal

DOCUMENT TYPE: LANGUAGE: English

OTHER SOURCE(S): CASREACT 94:84008 Eleven imidazoles I (R = Ph, substituted Ph, α -, β -naphthyl,

Structure-activity relationship was also discussed.

2-thienvl; R1 = H) were prepared by cyclizing RAc with quanidine using Br as condensing agent. Halogenating I (R1 = H) gave I (R1 = Br, C1). Both halogenated and nonhalogenated imidazoles exhibit antifungal activity against Piricularia oryzae and antibacterial activity against the common pathogenic bacteria, Staphylococcus aureus and Escherichia coli.

=> d 122 1-3 ibib ab hitstr

L22 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:80450 CAPLUS

DOCUMENT NUMBER: 140:145835

TITLE: Preparation of dibenzofused

bicvclo[2.2.2]octane-derived amides as modulators of

the glucocorticoid receptor

INVENTOR(S): Vaccaro, Wayne; Yang, Bingwei Vera; Kim, Soong-hoon; Huynh, Tram; Tortolani, David R.; Leavitt, Kenneth J.;

Li, Wenying; Doweyko, Arthur M.; Chen, Xiao-tao; Doweyko, Lidia

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA; et al.

PCT Int. Appl., 265 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

SOURCE:

WO 2004009017 A3 20040708 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD	
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD	CA. CH. CN.
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MX, MX, NI, NI PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ TR, TT, TZ, UA, UG, US, UZ, VC, VN, VU, ZA, ZM, ZW RW: GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK FT, FR, GB, GR, HU, LE, IT, LU, MC, NI, PT, RO, SE, SI	GD, GE, GH, LC, LK, LR, NO, NZ, OM, IJ, TM, TN, AM, AZ, BY, DK, EE, ES, SI, SK, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN AU 2003251970 A1 20040209 AU 2003-251970	
US 6995181 B2 20060207	
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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU JP 2006508042 T 20060309 JP 2004-523482 NO 2005000074 A 20050309 NO 2005-74 US 20050171136 A1 20050804 US 2005-85347 PRIORITY APPLN. INFO:: US 2003-621909 A1	HU, SK 20030717 20050106 20050321 20020718

OTHER SOURCE(S): MARPAT 140:145835 AB Title compds. I [R-R4 = H, alk(en/yn)yl, alkoxy, aryl, etc.; Z = carboxamido, alkylamino, etc.] are prepared For instance, 2-amino-4,5-dimethylthiazole is coupled to the acid derived from the cycloaddn. of methacrylic acid and anthracene (CH3CN, EDCI, Et3N, HOAt, 18 h) to give II. I are glucocorticoid receptor modulators which are useful in treating diseases requiring glucocorticoid receptor agonist or antagonist therapy such as obesity, diabetes, inflammatory and immune disorders. 650626-12-3 650626-16-7 RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of dibenzofused bicyclo[2.2.2]octane-derived amides as modulators of glucocorticoid receptor)

RN 650626-12-3 CAPLUS

CN 1H-Imidazol-2-amine, 5-(4-fluoro-1-naphthalenvl)- (CA INDEX NAME)

650626-16-7 CAPLUS RN

CN 1H-Imidazol-2-amine, 5-(6-methoxy-1-naphthalenyl)- (CA INDEX NAME)

L22 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:80449 CAPLUS

DOCUMENT NUMBER: 140:157927

TITLE: Homology modeling of nuclear hormone receptor Site II

and design of Site II ligands INVENTOR(S): Dowevko, Arthur; Nadler, Steven G.

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: PCT Int. Appl., 276 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	ENT				KIN		DATE				ICAT					ATE	
WO 2004009016																	
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		TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW			
	RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
		KG,	ΚZ,	MD,	RU,	ΤJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,
		FI,	FR,	GB,	GR,	HU,	IE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,
		BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
EP	1575	502			A2		2005	0921		EP 2	003-	7656	37		2	0030	717
EP	1575	502			A3		2005	1123									
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK	
US	2006	0223	110		A1		2006	1005		US 2	003-	6218	07		2	0030	717
RIT	APP	LN.	INFO	. :						US 2	002-	3969	07P	1	P 2	0020	718
										WO 2	003-	JS22	299	1	vi 2	0030	717

- AB A binding site in nuclear hormone receptors is described and its structural coordinates are provided. The invention provides machine-readable data storage media comprising structure coordinates of Site II and computer systems comprising the machine-readable data storage media. The invention provides methods used in the design and identification of ligands of Site II and of modulators of nuclear hormone receptors. The invention provides ligands of Site II, modulators of NHRs, pharmaceutical compns. comprising modulators of NHRs, methods of modulating NHRs, and methods of treating diseases by administering modulators of an NHR. Also provided are methods of designing mutants, mutant NHRs, Site II binding assays, and models of Site II.
- IIT 650626-12-38 650626-16-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(homol. modeling of nuclear hormone receptor Site II in ligand binding domain and design of Site II ligands)

RN 650626-12-3 CAPLUS

CN 1H-Imidazol-2-amine, 5-(4-fluoro-1-naphthalenyl)- (CA INDEX NAME)

PRI

RN 650626-16-7 CAPLUS

CN 1H-Imidazol-2-amine, 5-(6-methoxy-1-naphthalenyl)- (CA INDEX NAME)

L22 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2008 ACS on STN 1981:84008 CAPLUS

ACCESSION NUMBER: DOCUMENT NUMBER: 94:84008

ORIGINAL REFERENCE NO.: 94:13701a,13704a

TITLE: Synthesis and halogenation of some new

2-amino-4-substituted imidazoles and their possible

use as pesticides

AUTHOR(S): Nath, J. P.; Mahapatra, G. N.

Dep. Chem., Ravenshaw Coll., Cuttack, 753 003, India CORPORATE SOURCE: SOURCE: Indian Journal of Chemistry, Section B: Organic

Chemistry Including Medicinal Chemistry (1980)), 19B(6), 526-8

CODEN: IJSBDB; ISSN: 0376-4699 DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 94:84008

Eleven imidazoles I (R = Ph, substituted Ph, α -, β -naphthyl,

2-thienyl; R1 = H) were prepared by cyclizing RAc with quanidine using Br as condensing agent. Halogenating I (R1 = H) gave I (R1 = Br, C1). Both halogenated and nonhalogenated imidazoles exhibit antifungal activity against Piricularia oryzae and antibacterial activity against the common

pathogenic bacteria, Staphylococcus aureus and Escherichia coli. Structure-activity relationship was also discussed.

76507-28-3P 76507-39-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and pesticidal properties of)

RN 76507-28-3 CAPLUS

CN 1H-Imidazol-2-amine, 5-chloro-4-(1-naphthalenyl)- (CA INDEX NAME)

RN 76507-39-6 CAPLUS

1H-Imidazol-2-amine, 5-bromo-4-(1-naphthalenyl)- (CA INDEX NAME) CN

- IT 76507-18-1P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation, halogenation and pesticidal properties of) RN 76507-18-1 CAPLUS
- CN 1H-Imidazol-2-amine, 5-(1-naphthalenyl)- (CA INDEX NAME)